Низкоразмерные малочастичые системы в физике ультрахолодных квантовых газов

В.С.Мележик

ЛТФ ОИЯИ, Дубна

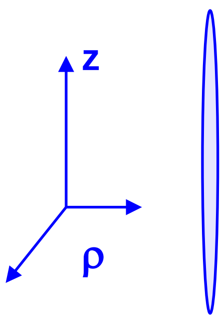
Дубна, 6-7 февраля 2014

Outline

- Quantum gas, what is this? Why it is interesting?
- Low-dimensional quantum systems in confining traps
- Theoretical models (pseudopotential approach)

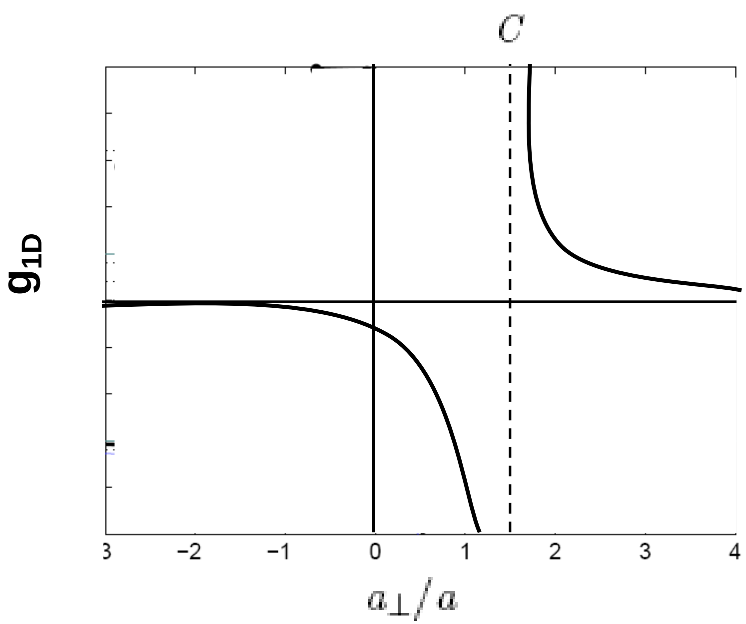
- Confinement-induced resonances in atomic traps
- Resonance mechanism of molecule formation in 1D trap with CM excitation
- Dipolar confinement-induced resonances
- “Fermionization of two distinguishable fermions”
- Outlook

Pseudopotential approximation in quasi-1D
("zero-range" potentials Yu.N.Demcov & V.N.Ostrovskii)



$$H_{1D} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} + g_{1D}\delta(z)$$

$$g_{1D} = \frac{2\hbar^2 a}{\mu a_\perp^2}\frac{1}{(1 - Ca/a_\perp)}$$



M.Olshanii,Phys.Rev.Lett. 81(1998)938

$$\hat{H} = \hat{H}_z + \hat{H}_\perp + \hat{V}$$

$$\hat{H}_z = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2}; \quad \hat{V}(\mathbf{r}) = \frac{2\pi\hbar^2 a}{\mu}\delta^3(\mathbf{r})$$

$$\hat{H}_\perp = -\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho}\right] + \frac{\mu}{2}\omega_\perp^2\rho^2$$

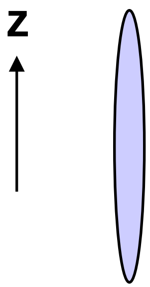
$$a_\perp = \sqrt{\frac{\hbar}{\mu\omega_\perp}}$$

$a_\perp / a = C$ **CIR**

$$C = 1.46\ldots$$

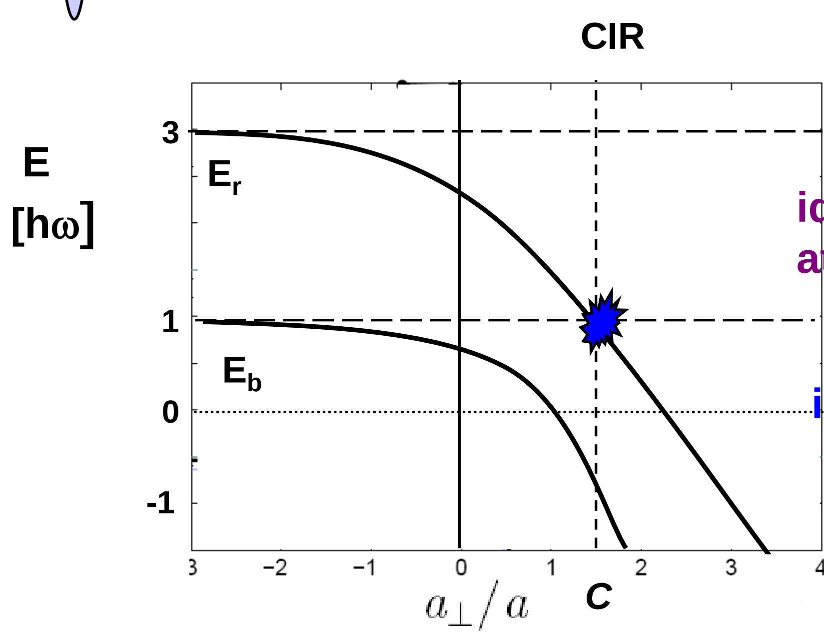
Pseudopotential approximation in quasi-1D (gas of impenetrable bosons at $a_\perp / a = C$)

$$g_{1D} = -\frac{\hbar^2}{\mu a_{1D}} = \frac{2\hbar^2 a}{\mu a_\perp^2} \frac{1}{(1 - Ca/a_\perp)} \underset{k \to 0}{=} \frac{\hbar^2 k \; Re\{f_0^+\}}{\mu \; Im\{f_0^+\}}$$



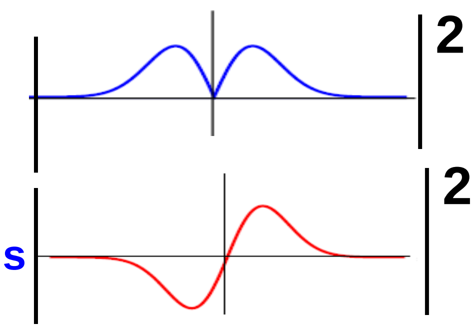
CIR: $g_{1D} \to \pm\infty \quad a_{1D} \to 0$ $\qquad f_0^+ = -\frac{1}{1+ika_{1D}} \to -1$

$$T = | 1 + f_0^+ |^2 \to 0 \quad !!$$



identical bosons at $g_{1D} \to \pm\infty$

identical fermions



impenetrable bosons (Tonks&Girardeau 1960)

M.D. Girardeau, PRA 82, 011607(R) (2010)

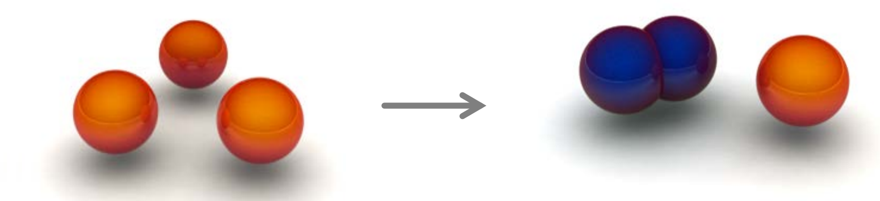
Experimental observation of CIR

T. Kinoshita, T. Wenger, D. S. Weiss, Science 305, 1125 (2004).
B. Paredes *et al.*, Nature 429, 277 (2004).

strongly-correlated Tonks-Girardeau gas

E. Haller *et al.*, Science 325, 1224 (2009)

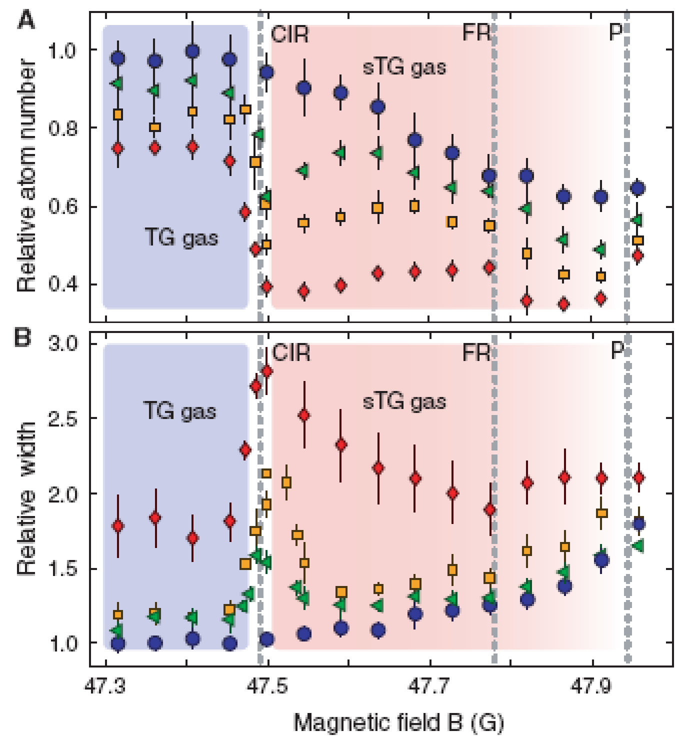
Detection of the CIR by an increase of three-body loss



three atoms → **molecule + atom**

in agreement with predicted CIR position

$$\frac{a_{3D}}{a_{\perp}} \approx 1$$

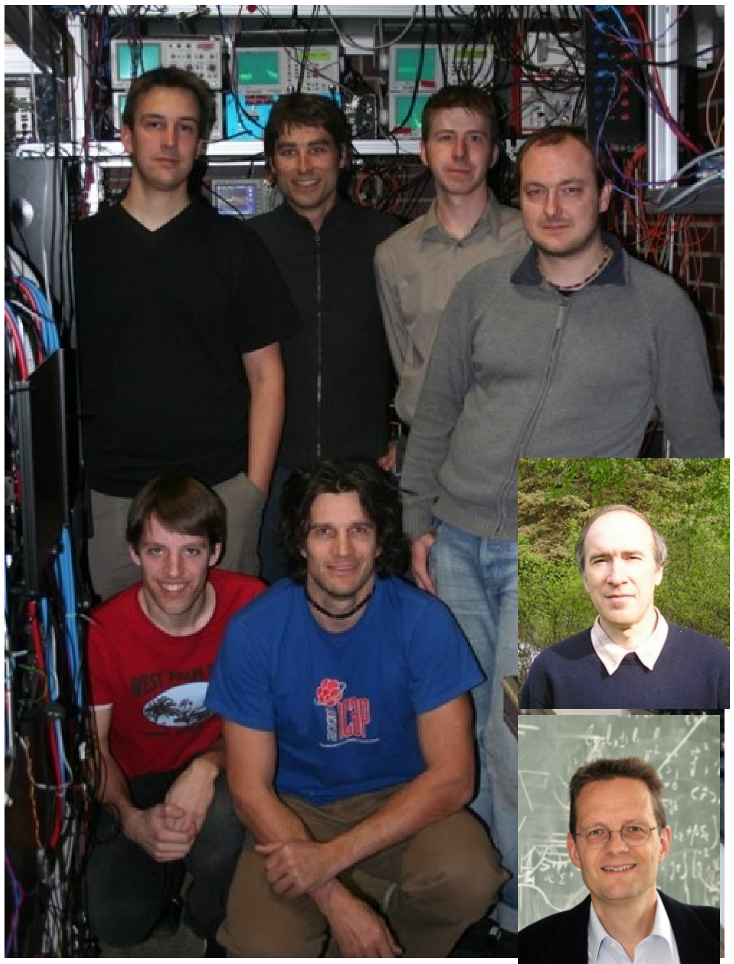


PRL **104,** 153203 (2010) PHYSICAL REVIEW LETTERS week ending 16 APRIL 2010

Confinement-Induced Resonances in Low-Dimensional Quantum Systems

Elmar Haller,[1] Manfred J. Mark,[1] Russell Hart,[1] Johann G. Danzl,[1] Lukas Reichsöllner,[1] Vladimir Melezhik,[2] Peter Schmelcher,[3] and Hanns-Christoph Nägerl[1]

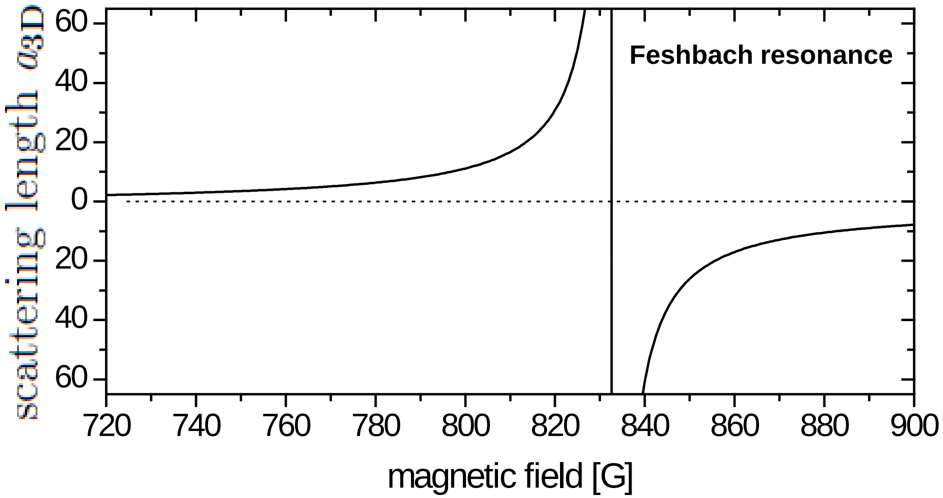
[1]*Institut für Experimentalphysik and Zentrum für Quantenphysik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria*
[2]*Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, 141980 Dubna, Russia*
[3]*Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany*
(Received 19 February 2010; published 14 April 2010)



In experiment performed in Innsbruck in collaboration with theoreticians from JINR and Hamburg, properties of ultracold Cs were studied by measuringthe atom loss in a 2D lattice formed by two retro-reflected laser beams

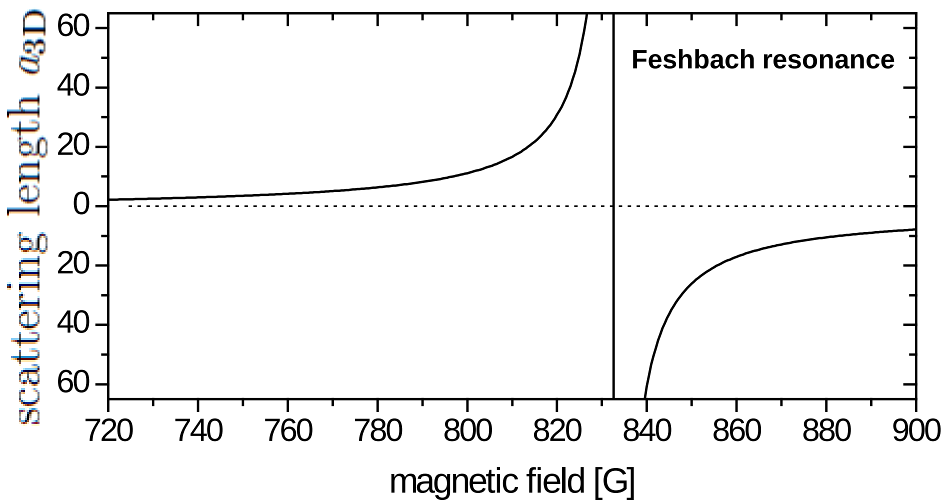
Tuning the interaction in 3D

3D



Tuning the interaction in 3D

3D

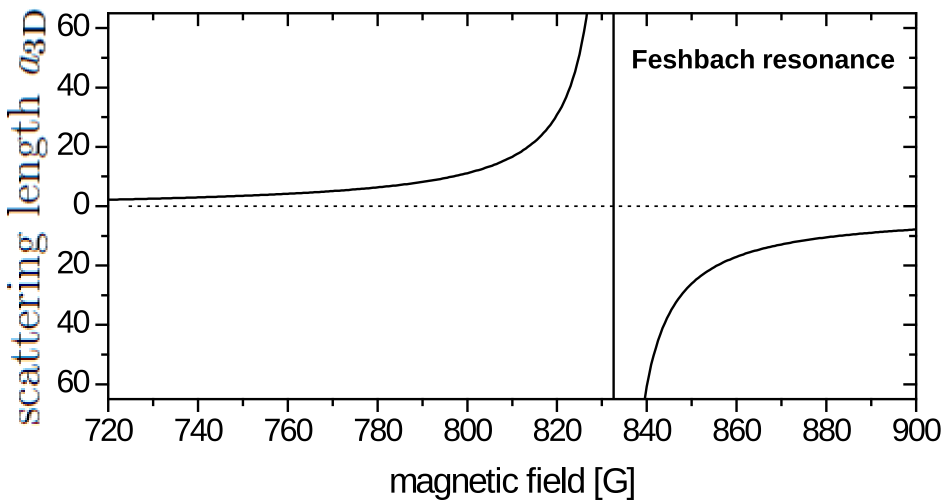


single-channel pseudopotential

$$\frac{2\pi\hbar^2 a_{3D}(B)}{\mu}\delta(\mathbf{r})$$

Tuning the interaction in 1D: B and ω

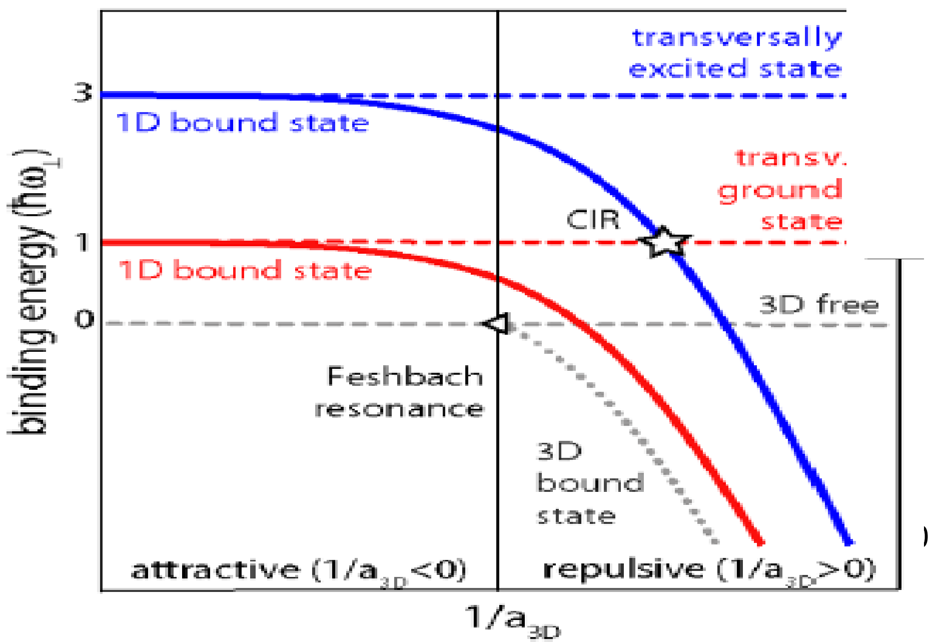
3D

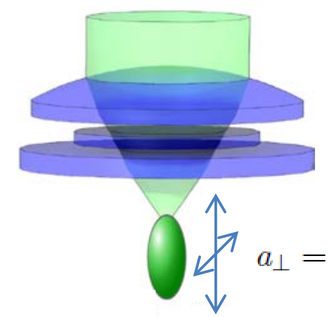


single-channel pseudopotential

$$\frac{2\pi\hbar^2 a_{3D}(B)}{\mu}\delta(\mathbf{r})$$

1D





$$a_\perp = \sqrt{\hbar/(\mu\omega)}$$

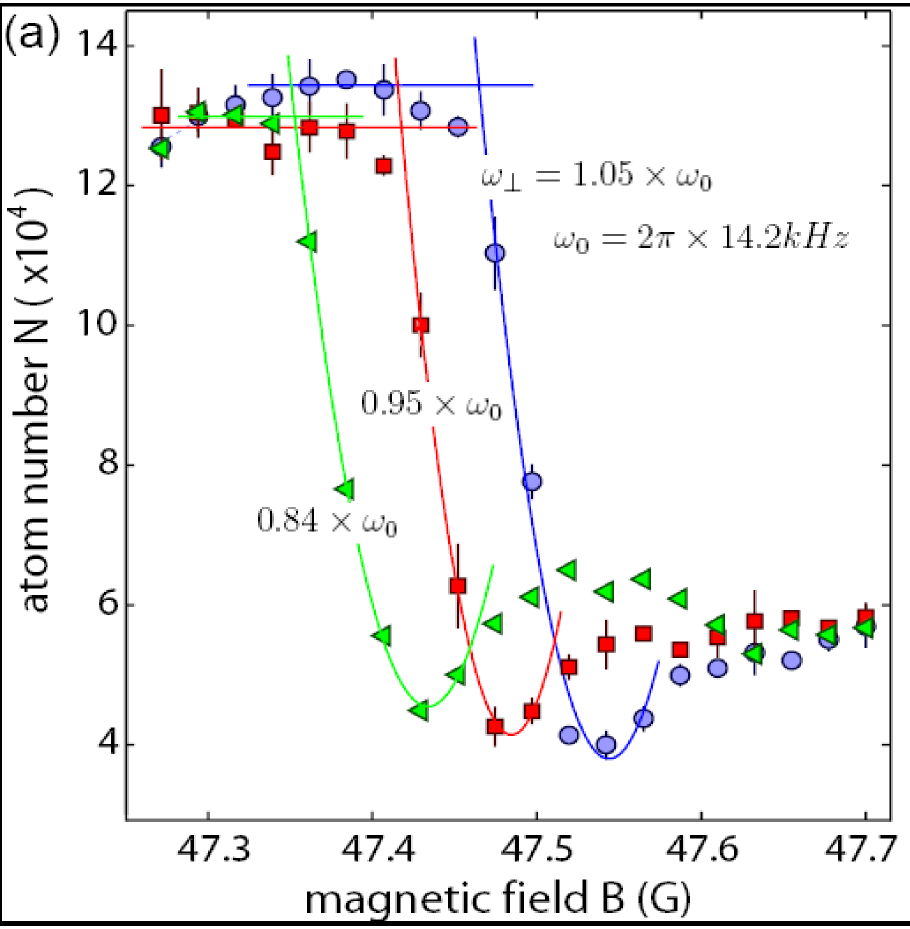
single-channel pseudopotential with renormalized interaction constant

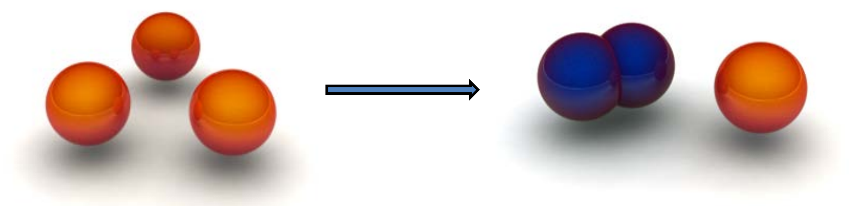
$$g_{1D} = \frac{2\hbar^2 a_{3D}(B)}{\mu a_\perp^2}\frac{1}{1 - C a_{3D}/a_\perp}$$

M. Olshanii, PRL 81, 938 (1998).

E.Haller, M.J. Mark, R. Hart, J.G. Danzl, L. Reichsoellner, V.Melezhik, P. Schmelcher and H.-C. Naegerle, Phys.Rev.Lett. 104 (2010)153203

isotropic traps $\omega_1 = \omega_2 = \omega_\perp$





three atoms **molecule + atom**

E.Haller, M.J. Mark, R. Hart, J.G. Danzl, L. Reichsoellner, V.Melezhik, P. Schmelcher and H.-C. Naegerle, Phys.Rev.Lett. 104 (2010)153203

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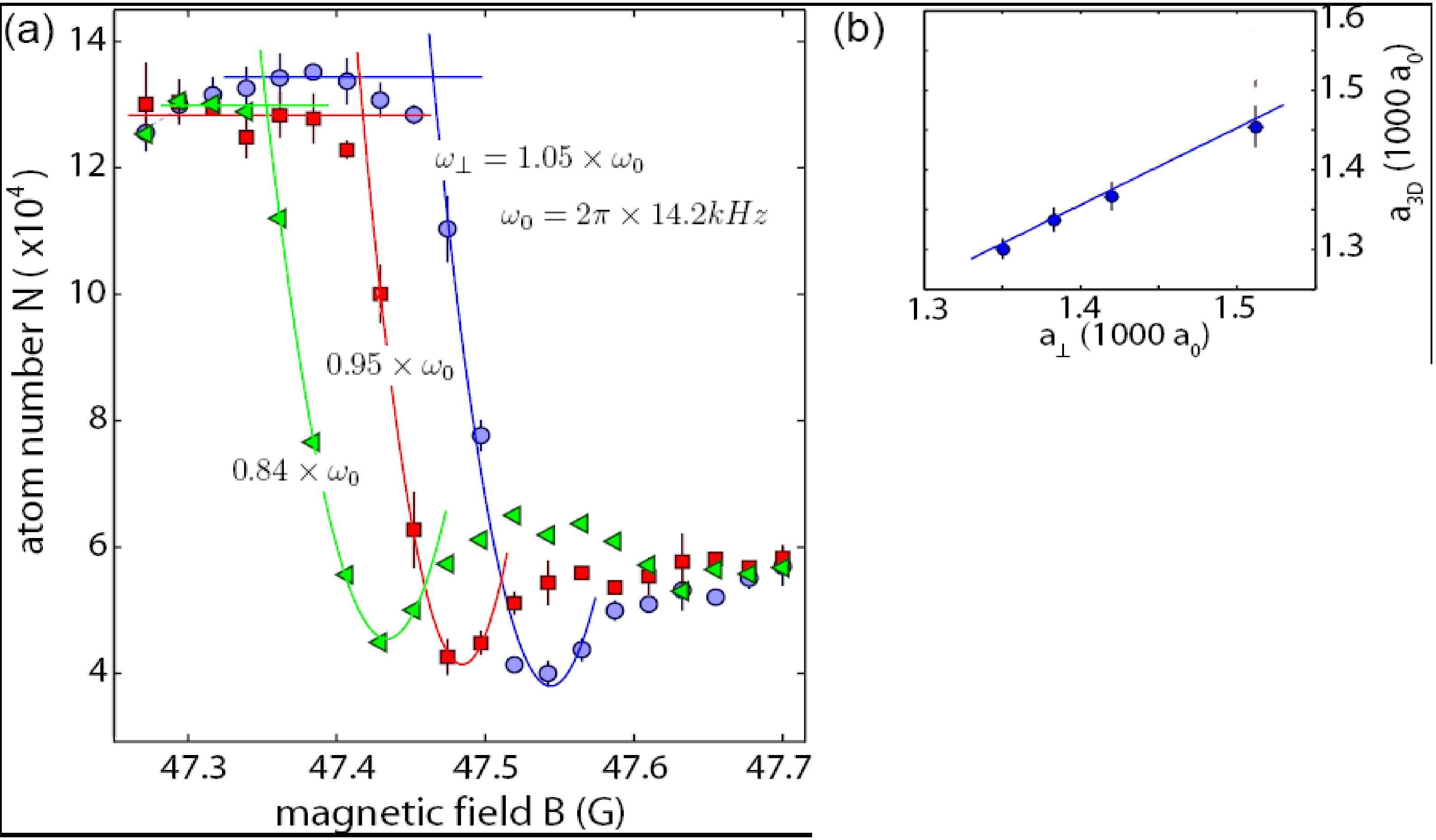


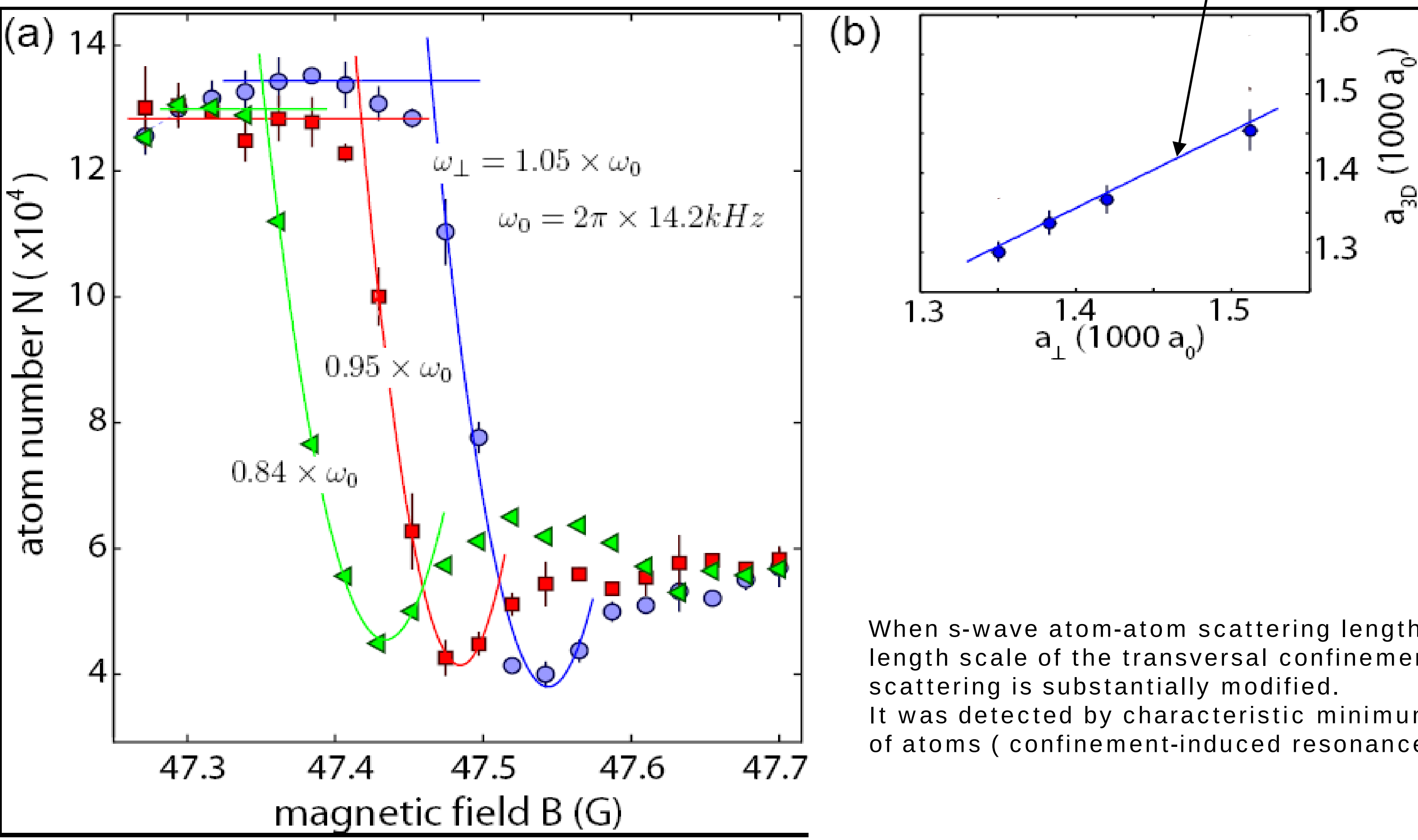
E.Haller, M.J. Mark, R. Hart, J.G. Danzl, L. Reichsoellner, V.Melezhik, P. Schmelcher and H.-C. Naegerle, Phys.Rev.Lett. 104 (2010)153203

isotropic traps $\omega_1 = \omega_2 = \omega_\perp$

$a_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}}$

$Ca_{3D} = a_\perp$ $\quad C_{theor} = 1.0326$

$C_{exp} = 1.0326$



When s-wave atom-atom scattering length approaches the length scale of the transversal confinement, atom-atom scattering is substantially modified.
It was detected by characteristic minimum of the number of atoms (confinement-induced resonance) in the 1D tubes

tensorial structure of the interatomic interaction V(r)

Feshbach Resonanzen

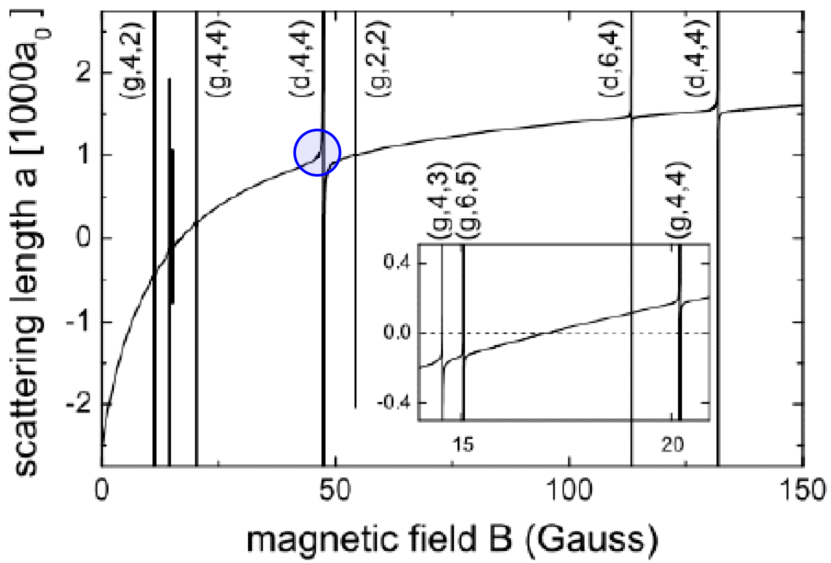
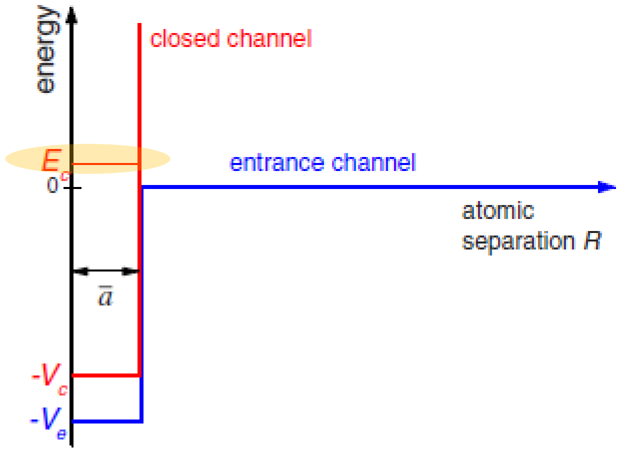


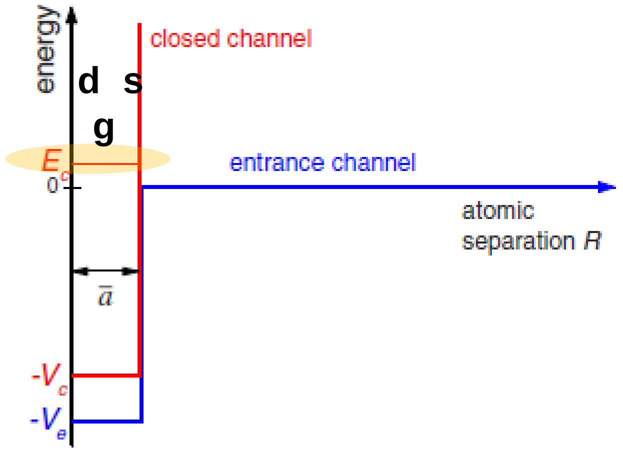
Figure 2.7.: Scattering length as a function of magnetic field for the state $F = 3$, $m_F = 3$. There is a Feshbach resonance at 48.0 G due to coupling to a d-wave molecular state. Several very narrow resonances at 11.0, 14.4, 15.0, 19.9 and 53.5 G are visible, which result from coupling to g-wave molecular states. The quantum numbers characterizing the molecular states are indicated, here as (l, f, m_f).

two-channel problem



two-channel problem

tensorial sructure of molecular state



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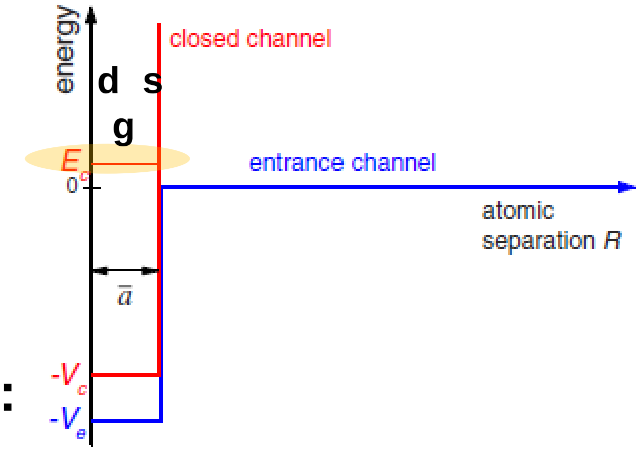
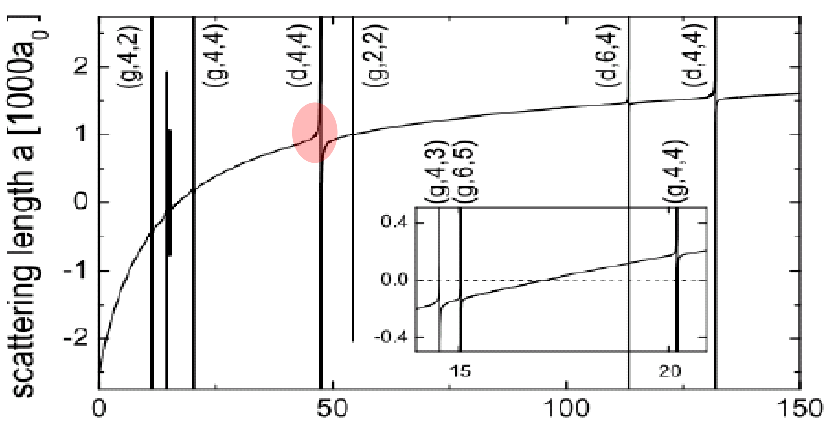


Innsbruck experiment with Cs atoms:

Feshbach Resonanzen

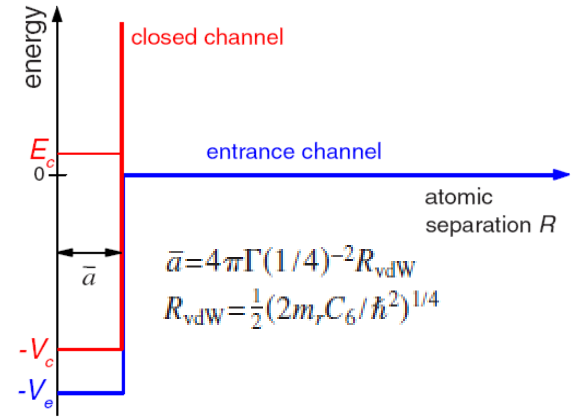


$$\mathbf{V}(\mathbf{r}) = \frac{2\pi\hbar^2 a}{\mu}\delta^3(r)$$

two-channel model of Lange et. al. Phys.Rev.79,013622(2009)

$$\hat{H}(r) = -\frac{\hbar^2}{2\mu}\hat{I}\frac{d^2}{d^2 r} + \hat{V}(r)$$

$$\hat{V} = \begin{bmatrix} -V_c & \hbar\Omega \\ \hbar\Omega & -V_e \end{bmatrix} \quad (\text{for } R < \bar{a}) = \begin{bmatrix} \infty & 0 \\ 0 & 0 \end{bmatrix} \quad (\text{for } R > \bar{a})$$



3 fitting parameters:

$$\frac{1}{a-\bar{a}} = \frac{1}{a_{\rm bg}-\bar{a}} + \frac{\Gamma/2}{\bar{a}E_c}$$

$$E_c = \delta\mu(B - B_c)$$

→ $V_e \; V_c \; \Omega$

$$\Gamma = \delta\mu\Delta$$

TABLE I. Fitting parameters for the s-, d-, and g-wave Feshbach resonances, determining the scattering length in the magnetic-field range of interest; see Fig. 3. The background scattering length $a_{\rm bg}=1875a_0$, the mean scattering length of cesium, $\bar{a}=95.7a_B$, and the bare s-wave state magnetic moment $\delta\mu_1=2.50\mu_B$ [28] are set constant. Poles $B_{0,i}$ and zeros B_i^* of the scattering length are derived; see text. Uncertainties in the parentheses are statistical. The systematic uncertainty of the magnetic field is 10 mG.

Res.	Γ_i/h (MHz)	$\delta\mu_i/\mu_B$	$B_{c,i}$ (G)	$B_{0,i}$ (G)	B_i^* (G)
s-wv.	11.6(3)	2.50	19.7(2)	−11.1(6)	18.1(6)
d-wv.	0.065(3)	1.15(2)	47.962(5)	47.78(1)	47.944(5)
g-wv.	0.0042(6)	1.5(1)	53.458(3)	53.449(3)	53.457(3)

extension of
two-channel model of Lange et. al. to 1D geometry

Sh.Saeidian, V.S. Melezhik ,and P.Schmelcher, Phys.Rev. A86, 062713 (2012)

A four-channel square-well potential

$$\hat{V} = \begin{pmatrix} -V_{c,3} & 0 & 0 & \hbar\Omega_3 \\ 0 & -V_{c,2} & 0 & \hbar\Omega_2 \\ 0 & 0 & -V_{c,1} & \hbar\Omega_1 \\ \hbar\Omega_3 & \hbar\Omega_2 & \hbar\Omega_1 & -V_e \end{pmatrix}$$

$$|\psi\rangle = \sum_\alpha \psi_\alpha(\mathbf{r})|\alpha\rangle = \sum_\alpha \phi_\alpha(r) Y_{l_\alpha 0}(\hat{r})|\alpha\rangle$$

$\omega_\perp = 0$

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l_\alpha(l_\alpha+1)}{2\mu r^2} + B_{\alpha\alpha}\right]\phi_\alpha(r) + \sum_\beta V_{\alpha\beta}(r)\phi_\beta(r) = E\phi_\alpha(r)$$

4-coupled radial equations

$$\psi_e(\mathbf{r}) \to \exp\{ikz\} + f(k,\theta)/r \; \exp\{ikr\}, \qquad \psi_{c,i}(\mathbf{r}) \to 0$$

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$$\left(\left[-\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega_\perp^2\rho^2\right]\hat{I} + \hat{B} + \hat{V}(r)\right)|\psi\rangle = E|\psi\rangle$$

4-coupled 2D equations in the plane $\{r, \theta\}$

$$\psi_e(\mathbf{r}) = [\cos(k_0 z) + f_e \exp\{ik_0|z|\}]\Phi_0(\rho), \quad \psi_{c,i}(\mathbf{r}) \to 0$$

$$T(B) = |1 + f_e(B)|^2$$

extension of two-channel model of Lange et. al. to 1D geometry

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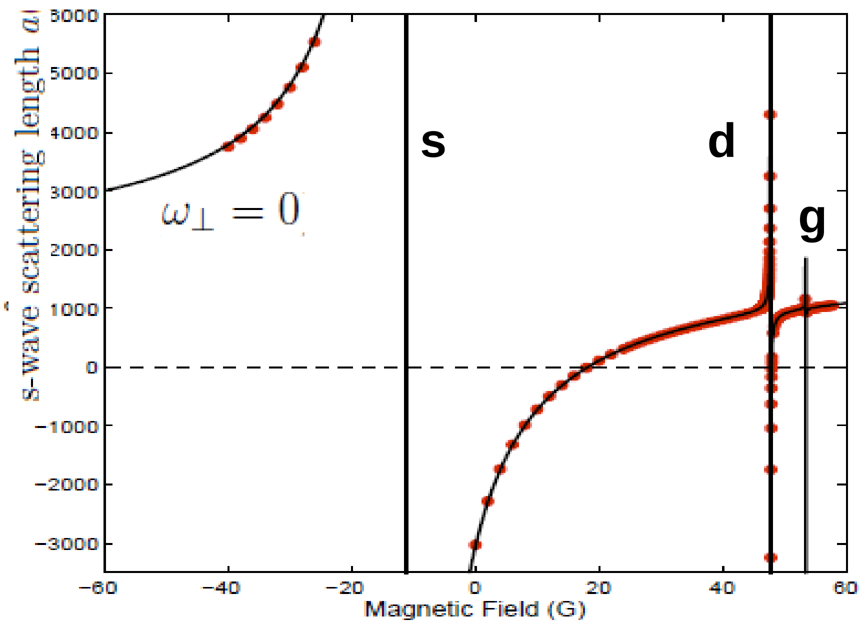
scattering problem → boundary-value problem

V.Melezhik,C.Y.Hu,Phys.Rev.Lett.90(2003)083202
S.Saeidian,V.Melezhik,P.Schmelcher,Phys.Rev.A77(2008)042701

Shifts and widths of Feshbach resonances in atomic waveguides

Sh.Saeidian, V.S. Melezhik ,and P.Schmelcher, Phys.Rev. A86, 062713 (2012)



Feshbach resonances in the Cs ultracold gas in the 3D free space

$$H(r,\theta) = [-\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega_\perp^2\rho^2]\hat{I} + \hat{V}(r)$$

$$V = \begin{pmatrix} -V_{C_3} & 0 & 0 & \hbar\Omega_3 \\ 0 & -V_{C_2} & 0 & \hbar\Omega_2 \\ 0 & 0 & -V_{C_1} & \hbar\Omega_1 \\ \hbar\Omega_3 & \hbar\Omega_2 & \hbar\Omega_1 & -V_e \end{pmatrix}$$

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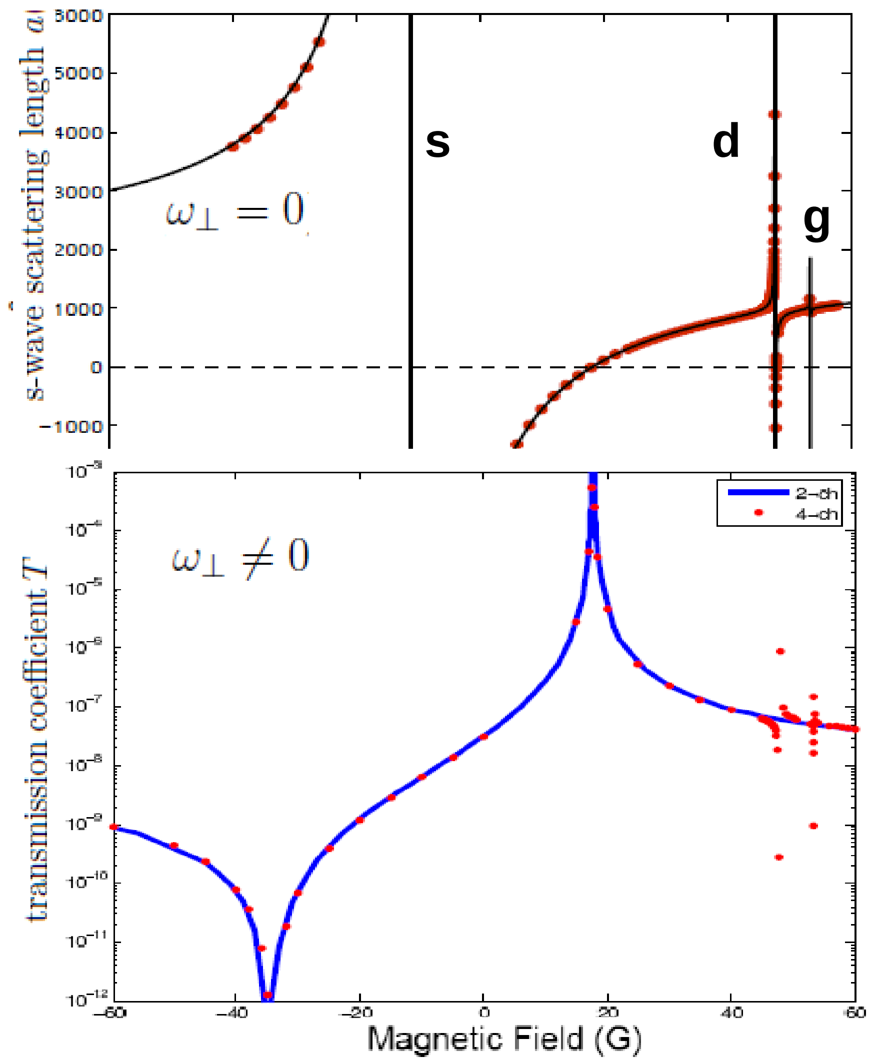

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in harmonic waveguides

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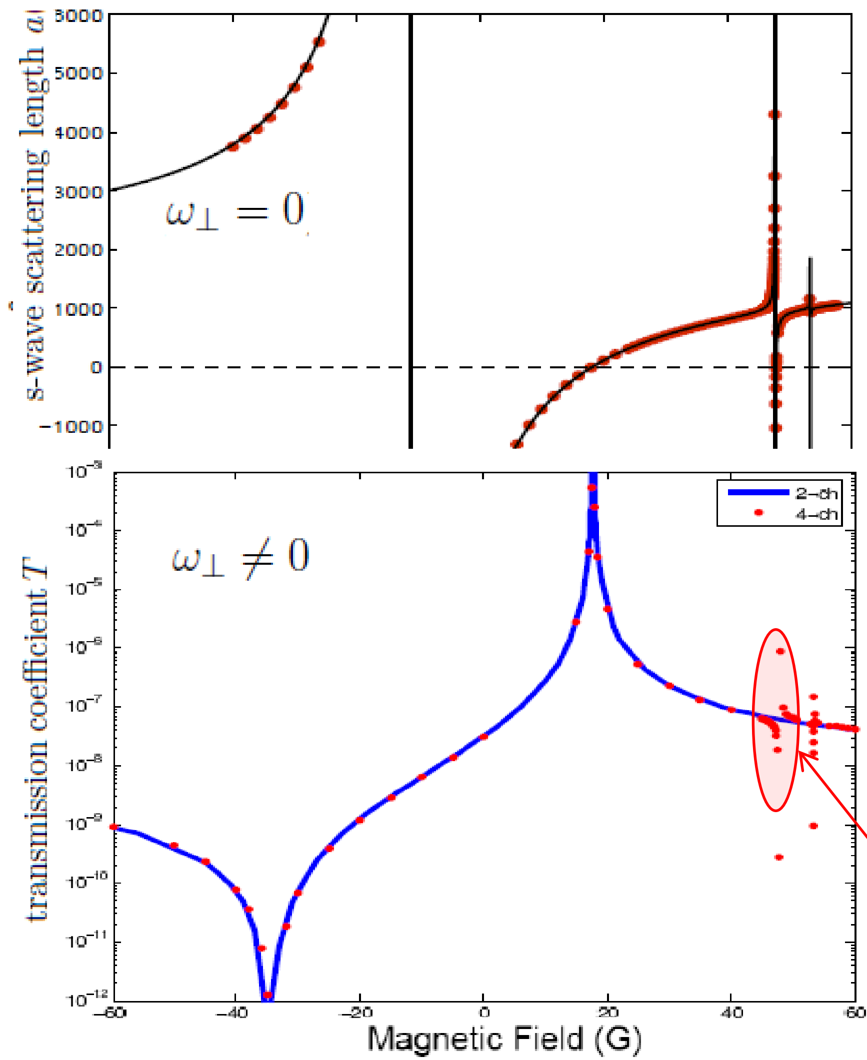

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in harmonic waveguides

region of Innsbruck experiment
(d-wave Feshbach resonance)

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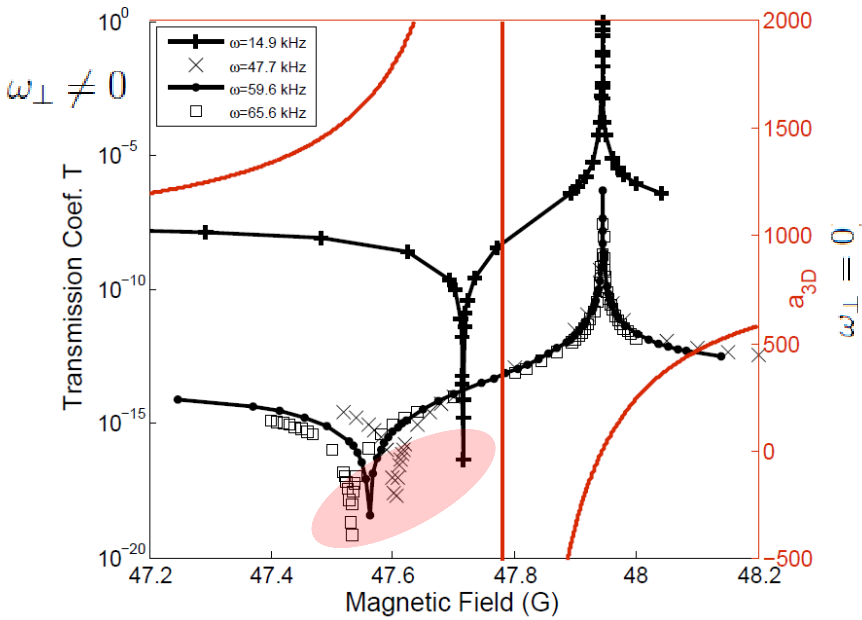

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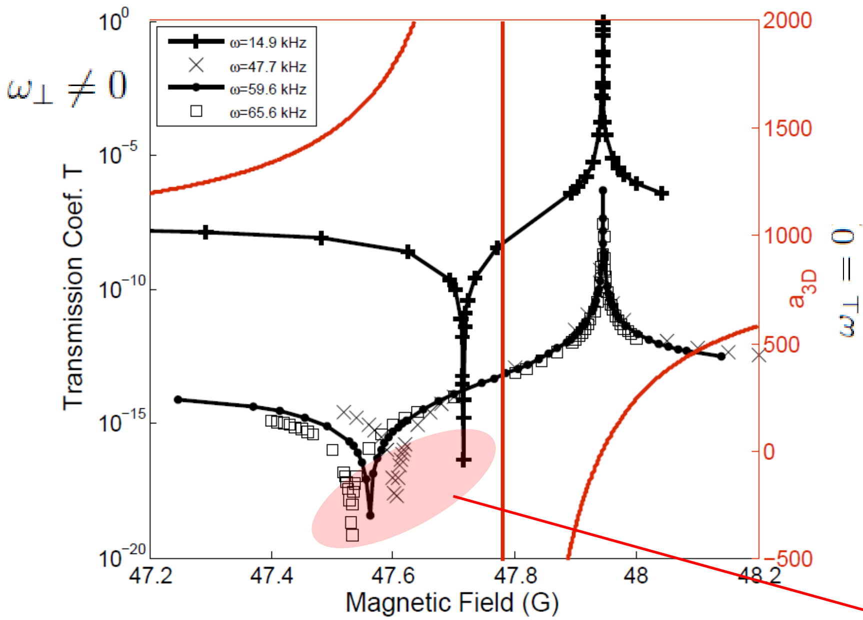

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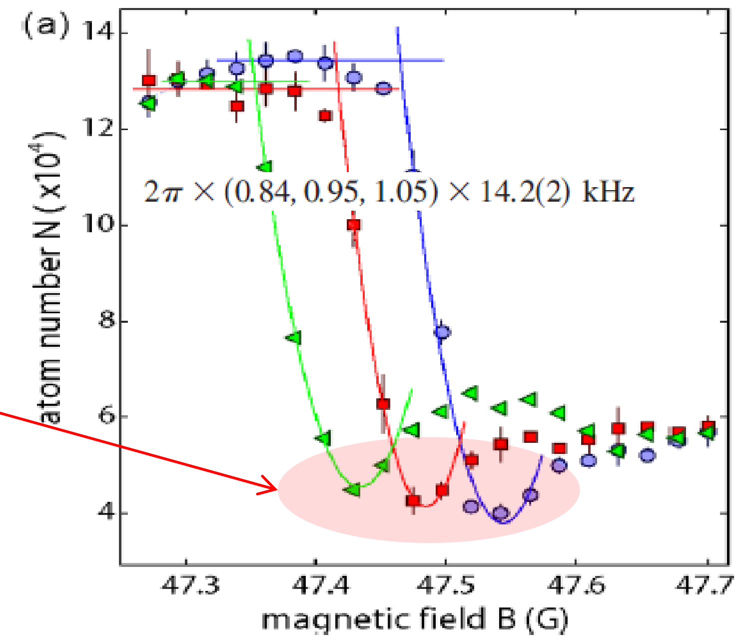

experiment:
E.Haller et.al. Phys.Rev.Lett.104, 153203 (2010)

Shifts and widths of Feshbach resonances in atomic waveguides

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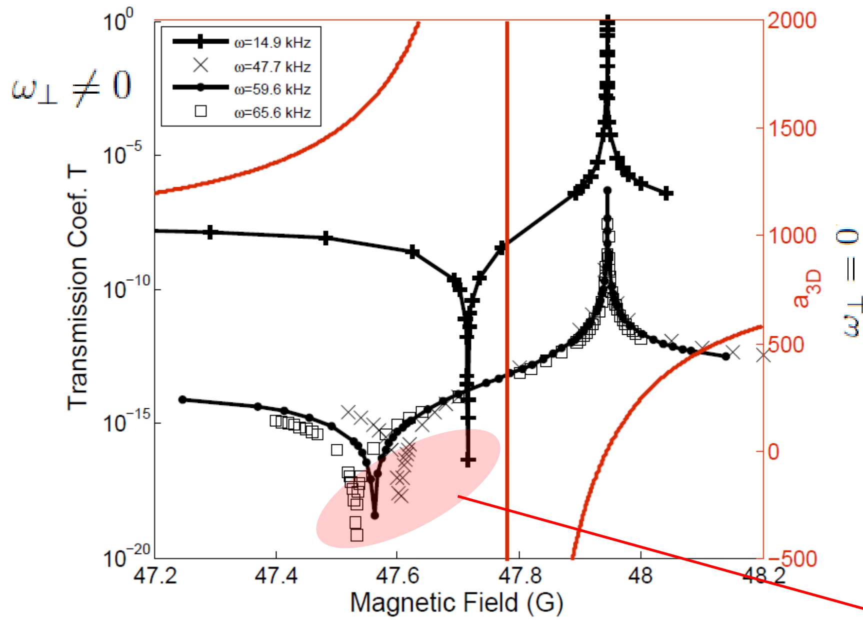
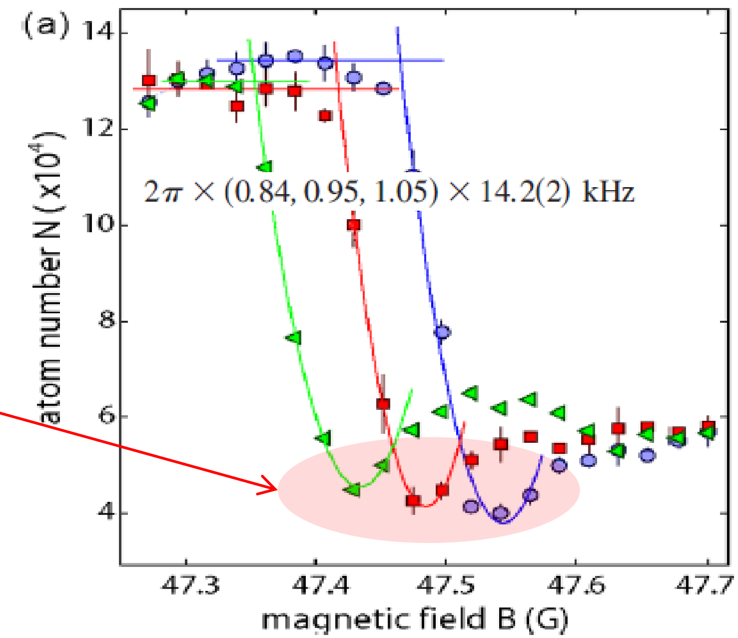
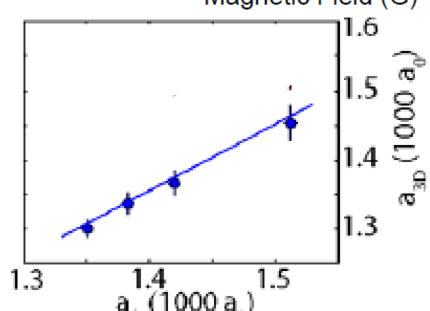


region of Innsbruck experiment
(d-wave Feshbach resonance)





$$a_{3D} = a_{3D}(B)$$

$$a_\perp = \sqrt{\frac{\hbar}{\mu\omega_\perp}}$$

our multi-channel theory coincides with single-channel theory of M.Olshanii, Phys.Rev.Lett.81,938 (1998) : $a_{3D} = 0.64 a_\perp$

experiment:
E.Haller et.al. Phys.Rev.Lett.104, 153203 (2010)

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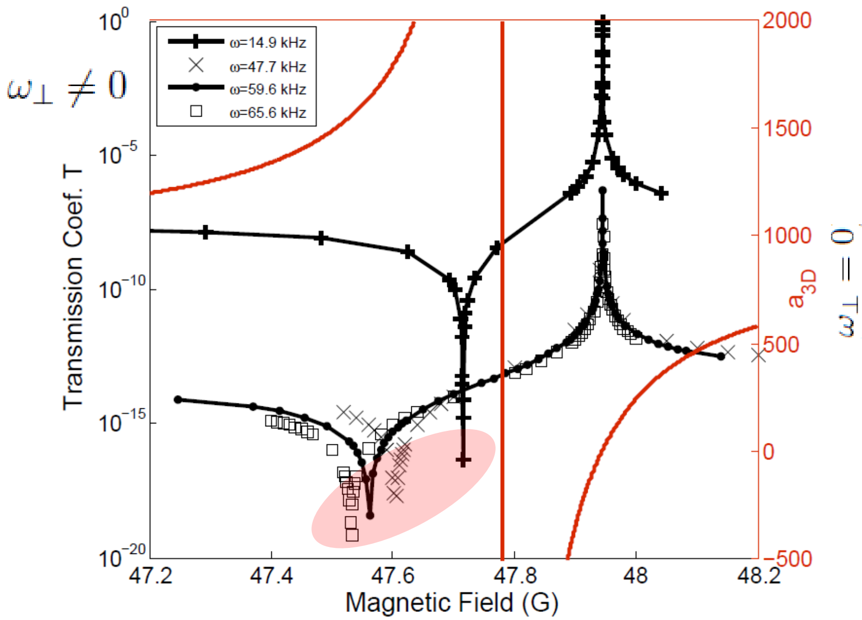

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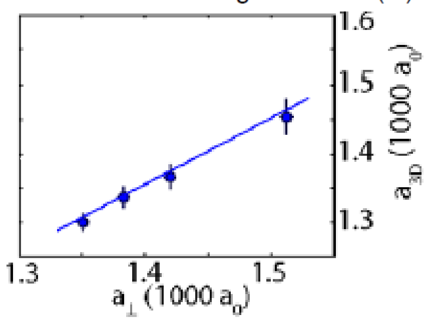

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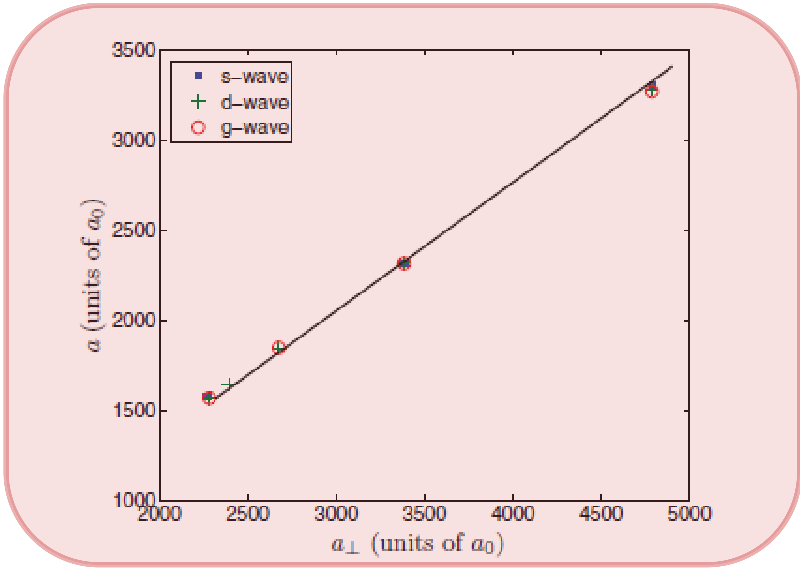

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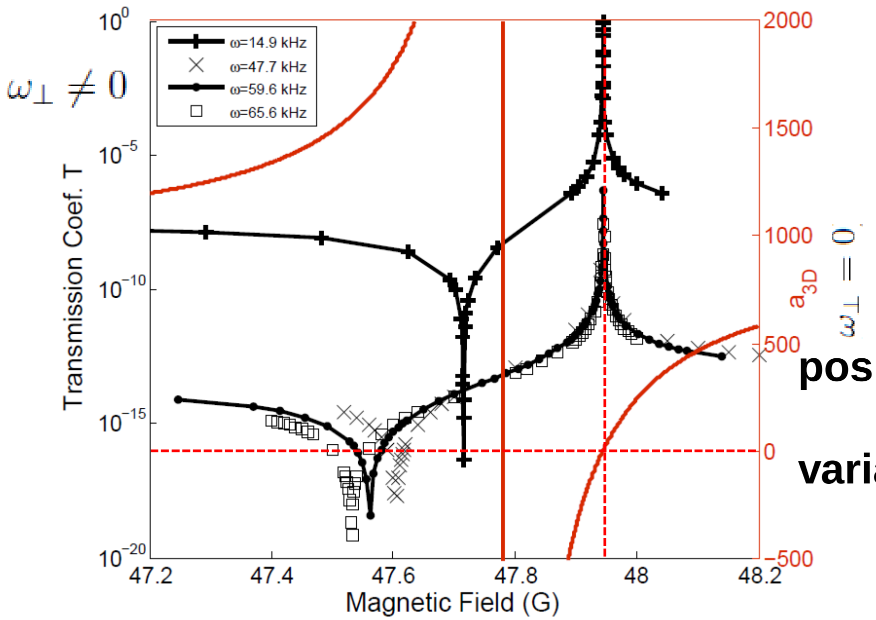

region of Innsbruck experiment

(d-wave Feshbach resonance)

position of T_{max} is stable with respect to variation of $\omega_\perp$ and coincides with $a_{3D} = 0$

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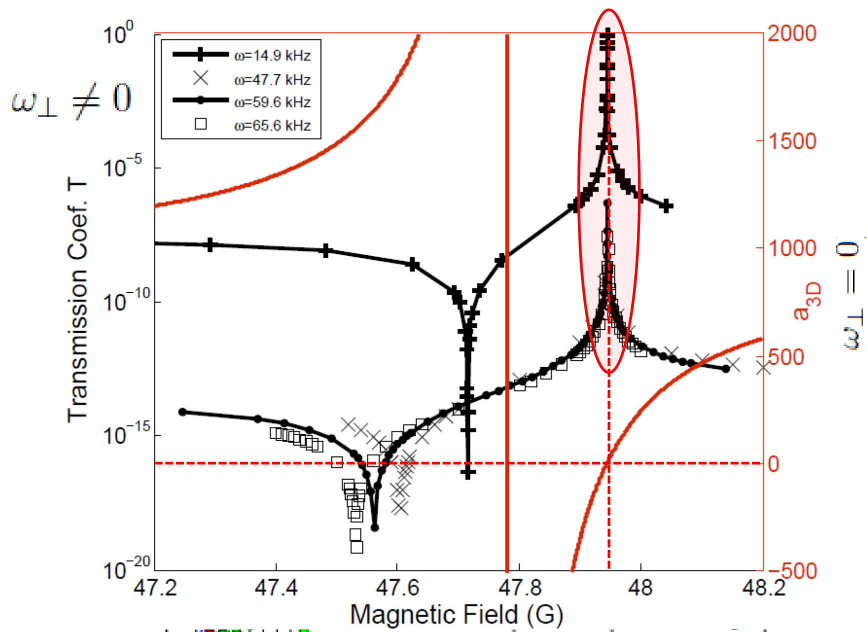

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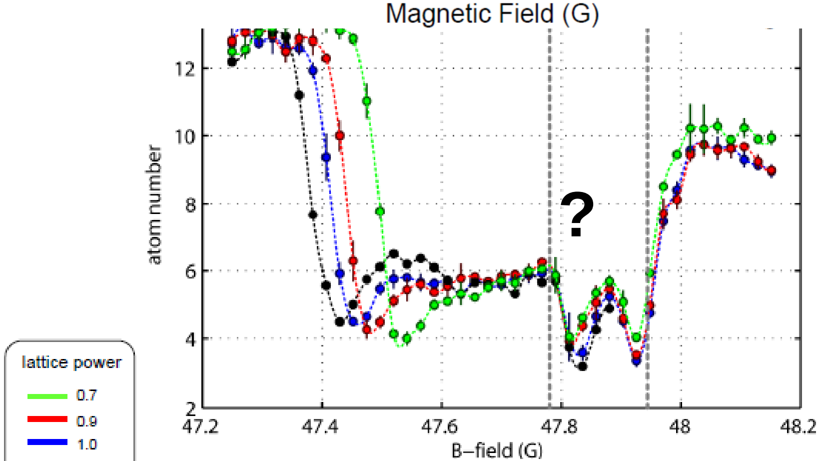

Innsbruck data, E.Haller (unpublished)

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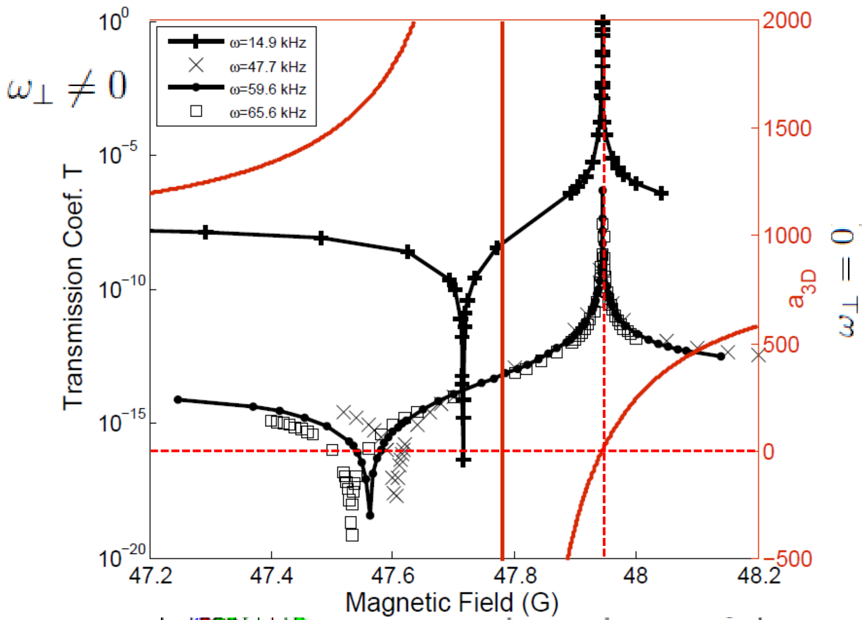

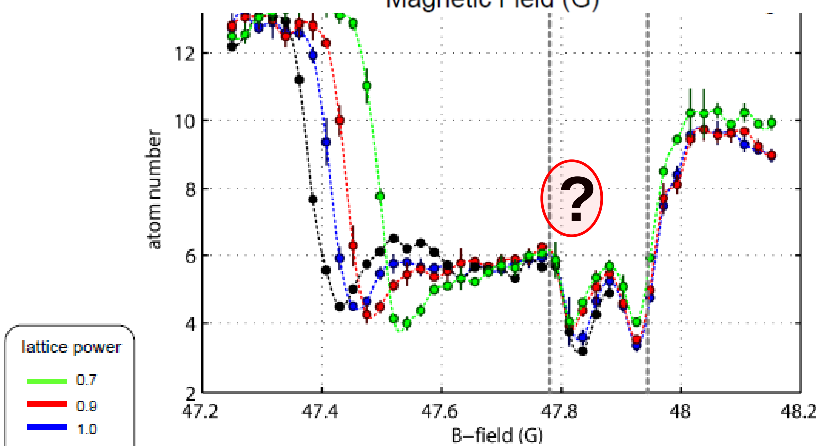

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?

1) **d-wave shape resonance**

2) **Efimov like resonance (3 body) :**

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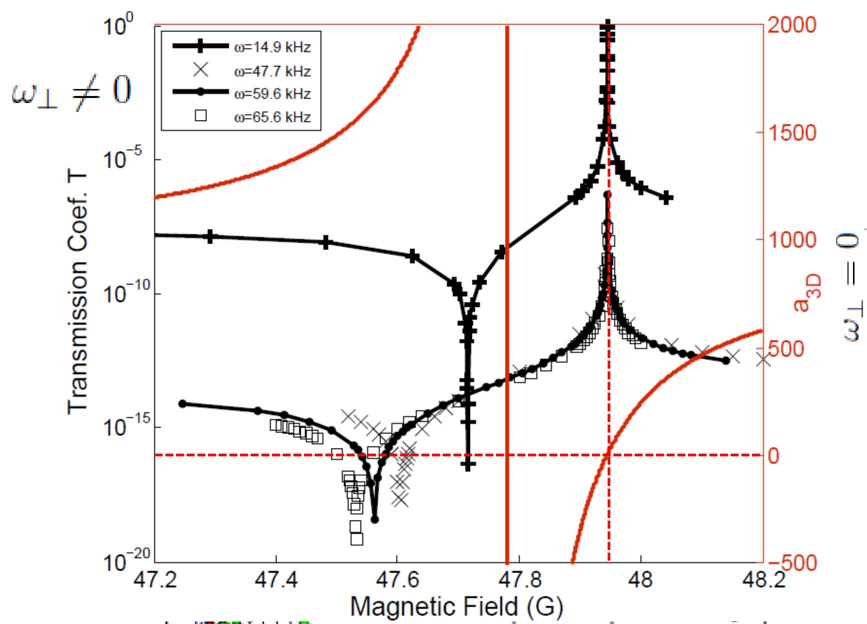
Sh.Saeidian, V.S. Melezhik ,and P.Schmelcher, Phys.Rev. A86, 062713 (2012)



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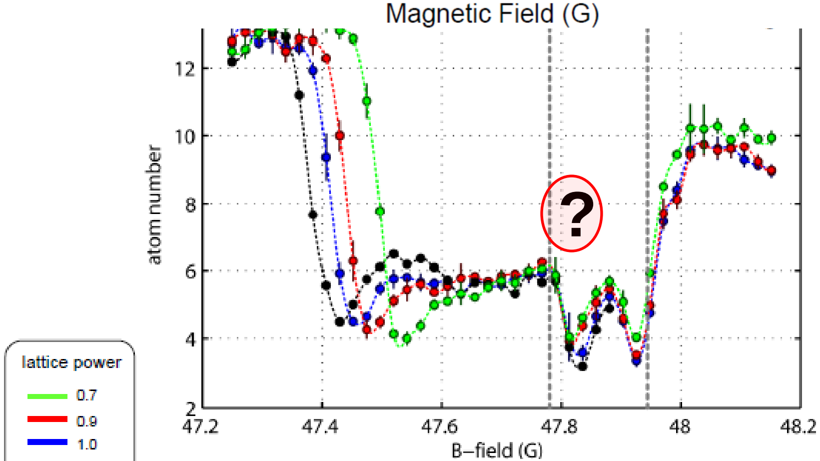

?

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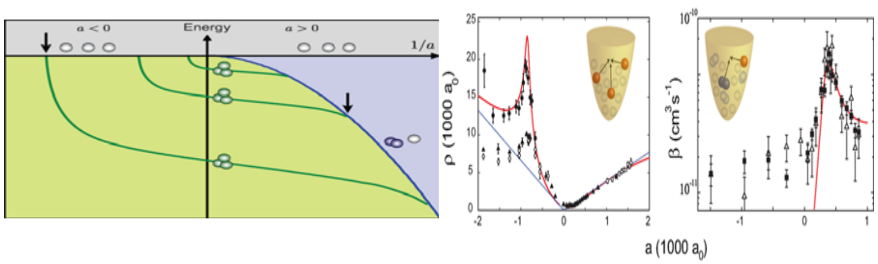
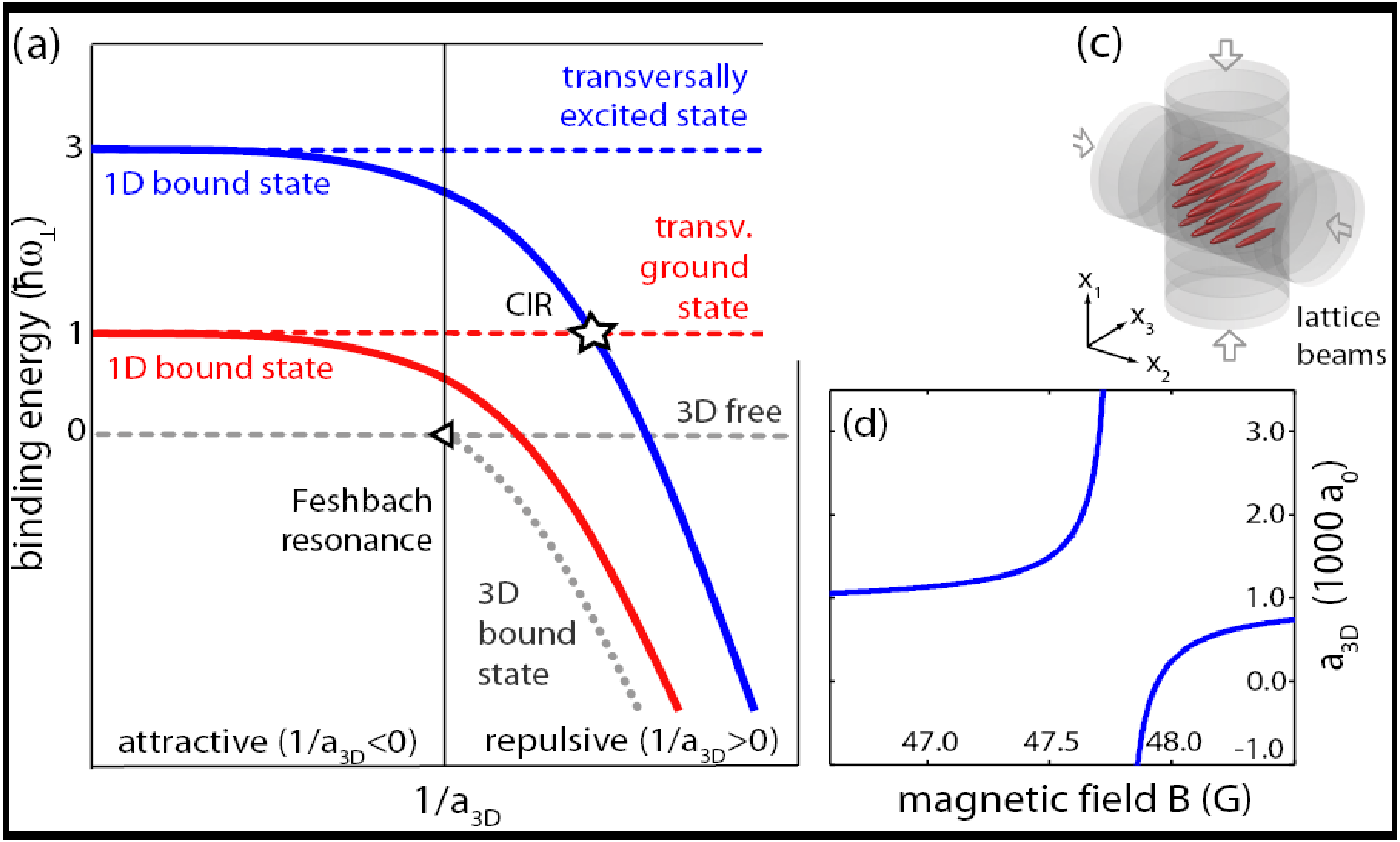


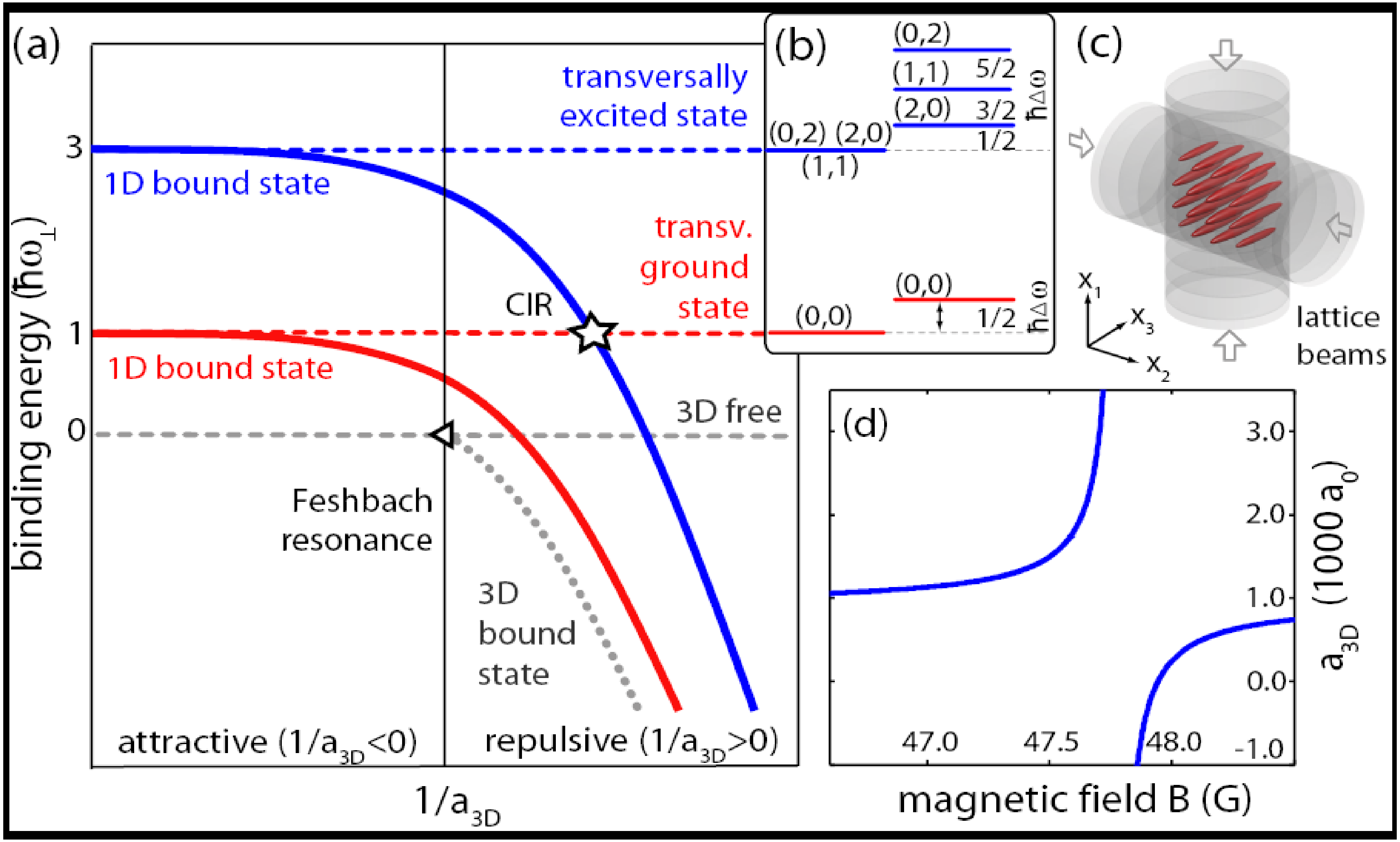
anisotropic traps $\omega_1 - \omega_2 = \Delta \neq 0$ **?**

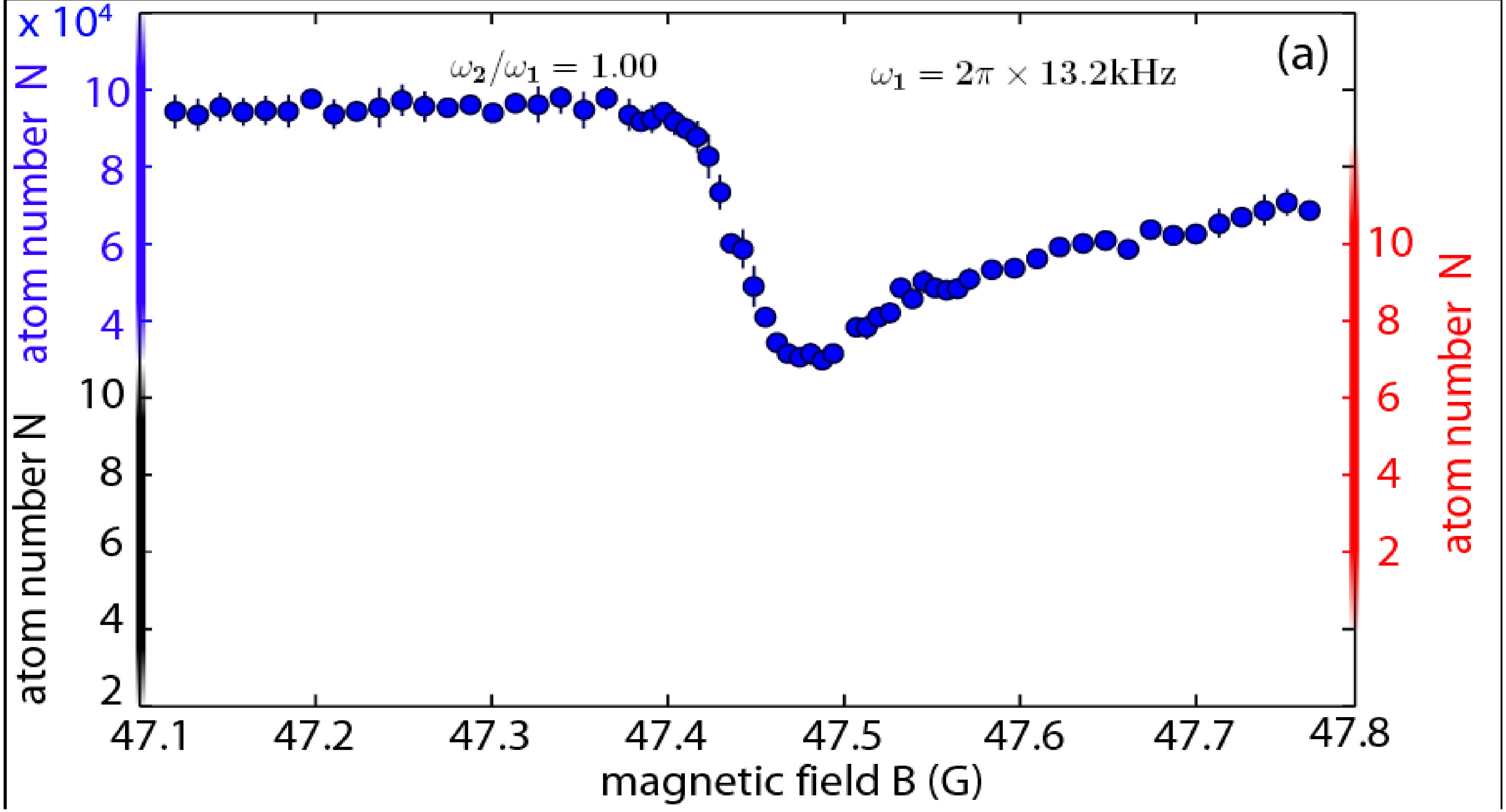


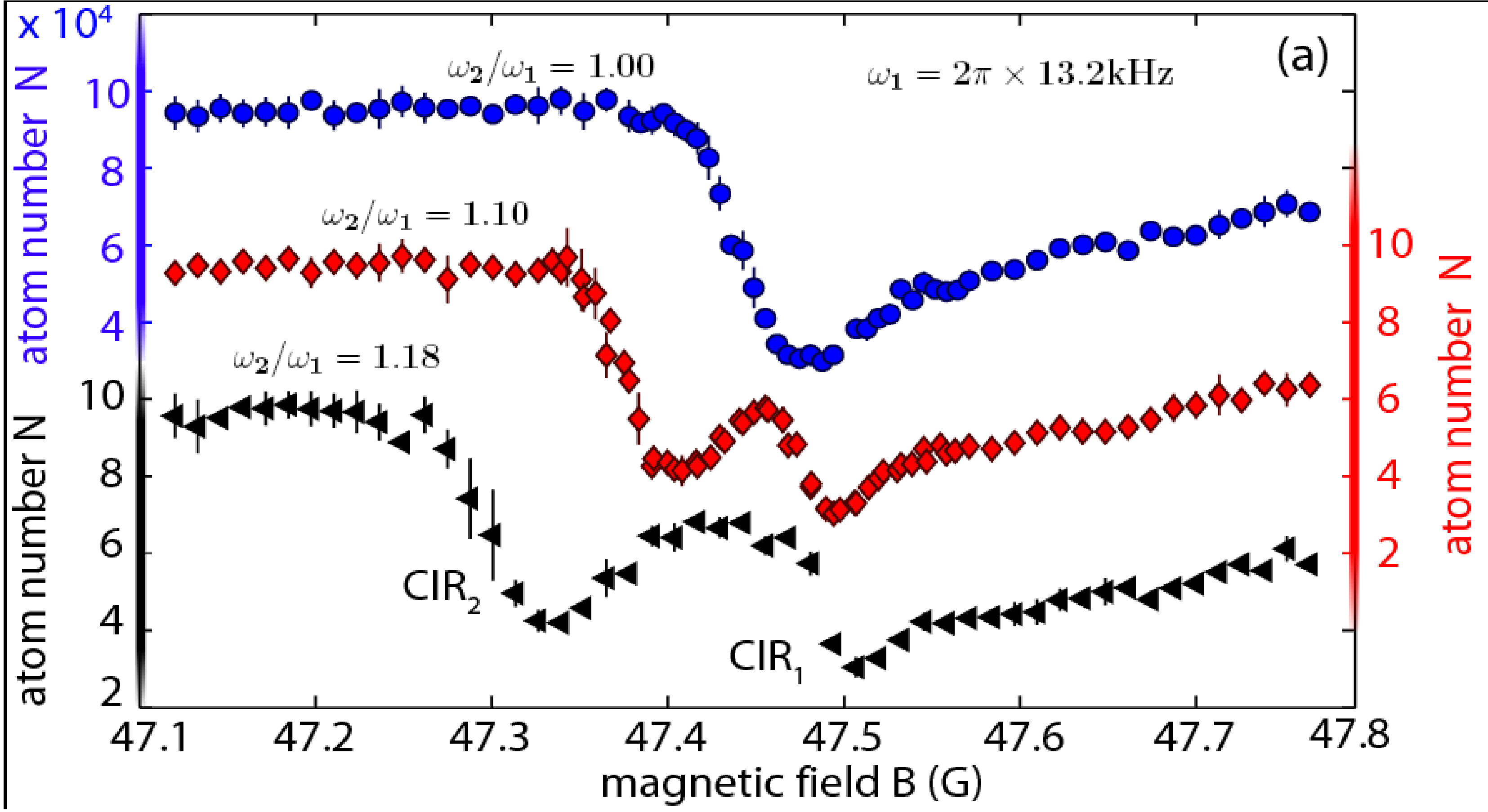
anisotropic traps $\omega_1 - \omega_2 = \Delta \neq 0$ **?**

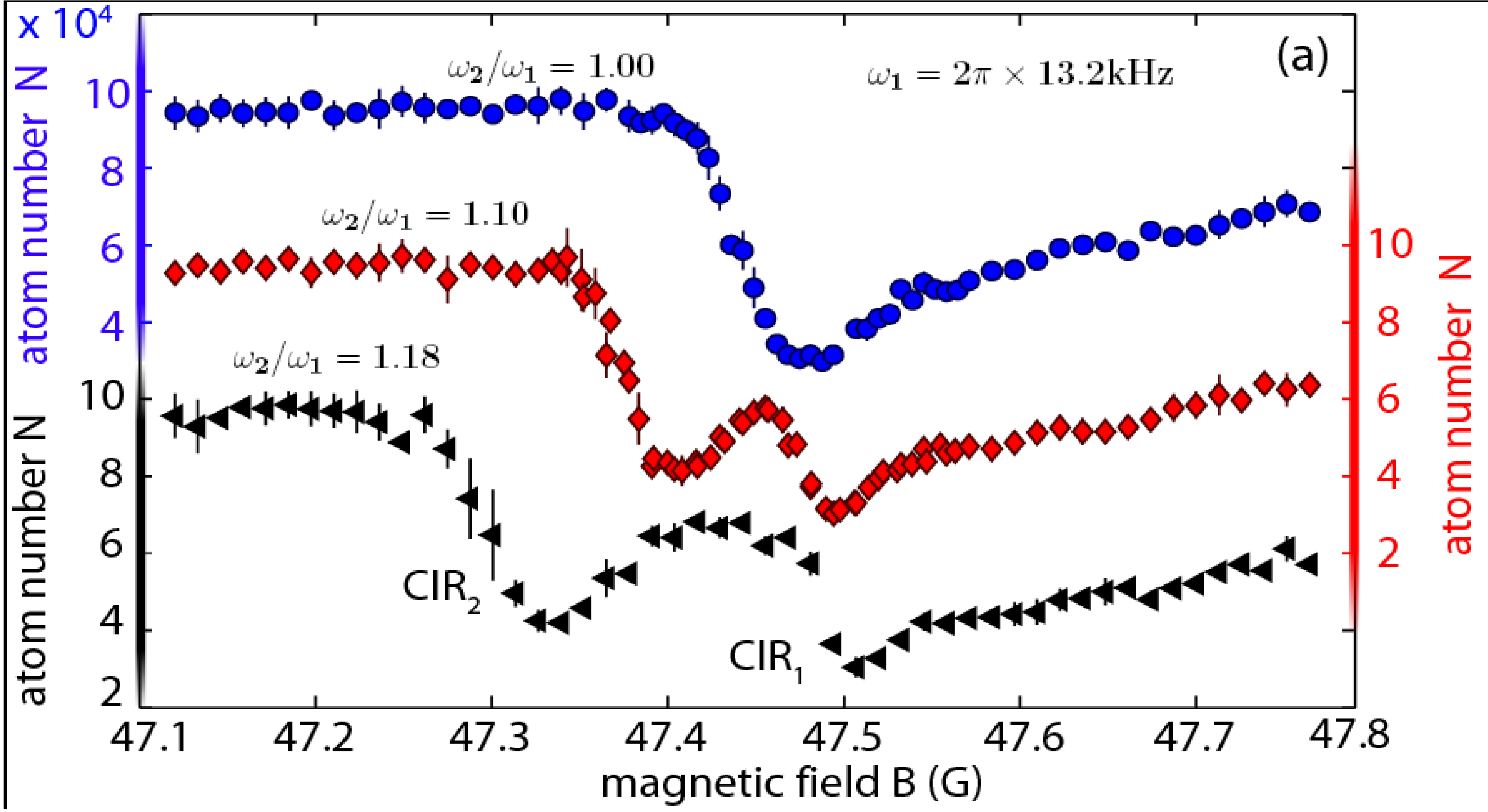
CIR splitting **!**

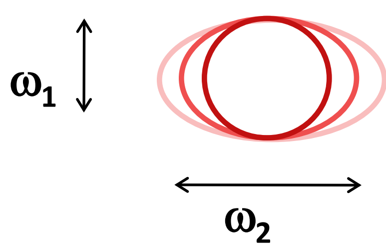
$$E_{n_1,n_2} = \hbar\omega_1(n_1 + n_2 + 1) + \hbar\Delta\omega(n_2 + \tfrac{1}{2})$$




x 10^4
atom number N
10
8
6
4
2
$\omega_2/\omega_1 = 1.00$
$\omega_1 = 2\pi \times 13.2$kHz
(a)
47.1
47.2
47.3
47.4
47.5
47.6
47.7
47.8
magnetic field B (G)


x 10^4
atom number N
atom number N
atom number N
$\omega_2/\omega_1 = 1.00$
$\omega_1 = 2\pi \times 13.2\text{kHz}$
(a)
$\omega_2/\omega_1 = 1.10$
$\omega_2/\omega_1 = 1.18$
CIR_2
CIR_1
magnetic field B (G)

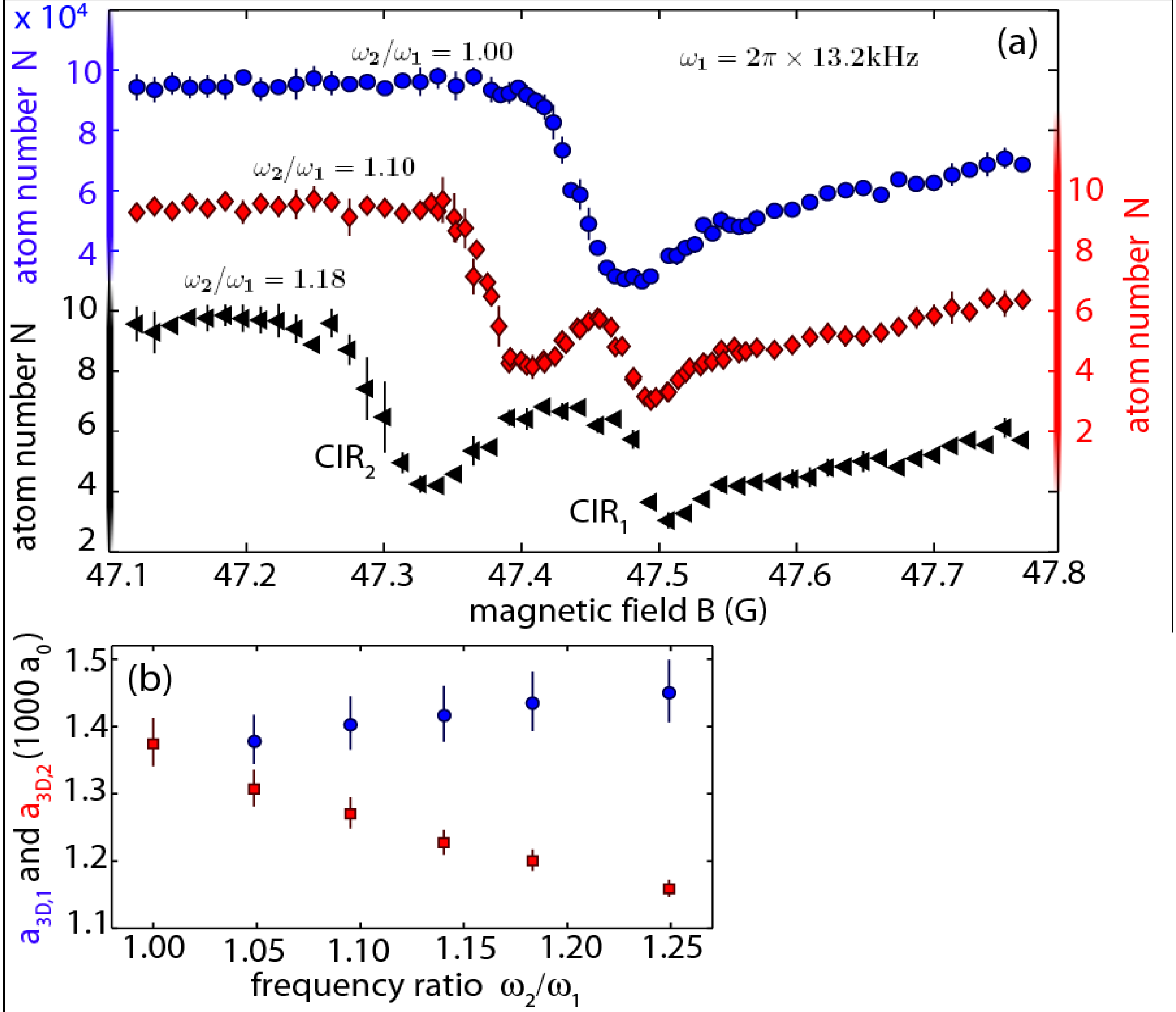




a splitting of the confinement-induced resonance
was found upon introducing an anisotropy
for the transversal confinement

anisotropic
transversal
confinement

a splitting of the confinement-induced resonance
was found upon introducing an anisotropy $\omega_1 \neq \omega_2$
for the transversal confinement



x 10^4
atom number N
$\omega_2/\omega_1 = 1.00$
$\omega_1 = 2\pi \times 13.2\text{kHz}$
(a)
$\omega_2/\omega_1 = 1.10$
$\omega_2/\omega_1 = 1.18$
atom number N
atom number N
CIR$_2$
CIR$_1$
magnetic field B (G)
47.1 47.2 47.3 47.4 47.5 47.6 47.7 47.8
(b)
$a_{3D,1}$ and $a_{3D,2}$ (1000 a_0)
frequency ratio ω_2/ω_1
1.00 1.05 1.10 1.15 1.20 1.25

Two attempts to describe the CIR splitting at $\omega_1 = \omega_2$ in pseudopotential approach

S.-G.Peng, S. Bohloul, X.J. Liu, H. Hu, P. Drummond, Phys.Rev.A82(2010)
W.Zhang, P.Zhang, Phys.Rev.A83(2011)

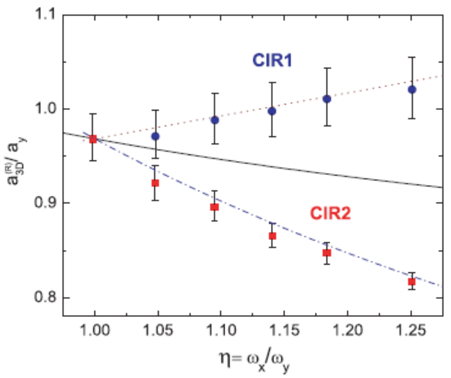
$$\mathcal{H}_{rel} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} + \mathcal{H}_\perp + g_{3D}\delta(\mathbf{r})\frac{\partial}{\partial r}r,$$

where $g_{3D} = 4\pi\hbar^2 a_{3D}/m$

$$\mathcal{H}_\perp = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}\mu\omega_y^2\left(\eta^2 x^2 + y^2\right)$$

$$\mathcal{H}_{1D} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} + g_{1D}\delta(z)$$

$$g_{1D} = \frac{2\hbar^2 a_{3D}}{\mu d^2}\frac{\sqrt{\eta}}{1 - \sqrt{\eta}\mathcal{C}(a_{3D}/d)}$$



no CIR splitting !

Multichannel scattering problem in harmonic waveguide (1D geometry)

Hamiltonian (atom-atom relative motion)

$$H(x,y,z) = -\frac{\hbar^2}{2\mu}\triangle_{\mathbf{r}} + \frac{1}{2}\mu\,\omega_1^2 x^2 + \frac{1}{2}\mu\,\omega_2^2 y^2 + V(r)$$

scattering wave function at $|\,z\,| \to +\infty$

$$\psi_{n_1,n_2}(\mathbf{r}) = \cos(k_{n_1,n_2} z)\phi_{n_1,n_2}(x,y) + \sum_{n'_1,n'_2=0}^{m_1,m_2} f_{n_1,n_2}^{n'_1,n'_2} \times \exp\{ik_{n'_1,n'_2}\,|\,z\,|\}\phi_{n'_1,n'_2}(x,y)\ .$$

$f_{n_1,n_2}^{n'_1,n'_2}(E)$ scattering amplitude describes transition

from $E_{\perp}^{(n_1,n_2)} = \hbar[\omega_1(n_1+\frac{1}{2}) + \omega_2(n_2+\frac{1}{2})]$

to $E = E_{\perp}^{(n'_1,n'_2)} + E'_{\|}$

V.Melezhik &P.Schmelcher, Phys.Rev.A84(2011)

Multichannel scattering problem in harmonic waveguide (1D geometry)

partial transmission coefficients

$$T_{n_1,n_2} = \sum_{n'_1,n'_2} \frac{k_{n'_1,n'_2}}{k_{n_1,n_2}} \mid \delta_{n_1,n'_1} \delta_{n_2,n'_2} + f_{n_1,n_2}^{n'_1,n'_2} \mid^2$$

describe transition probabilities

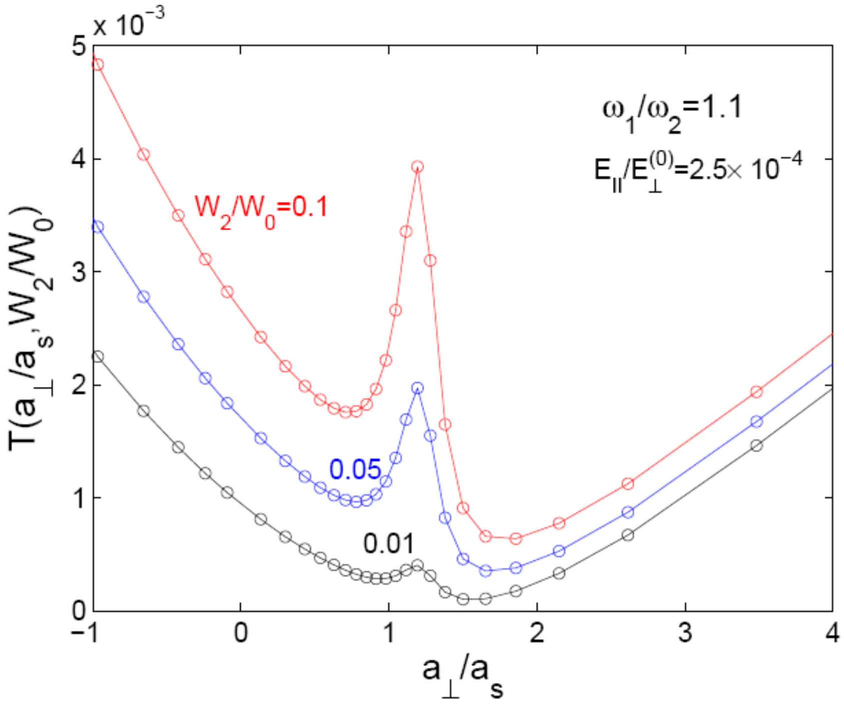
from initial transverse state (n_1, n_2)

to all possible final states (n'_1, n'_2)

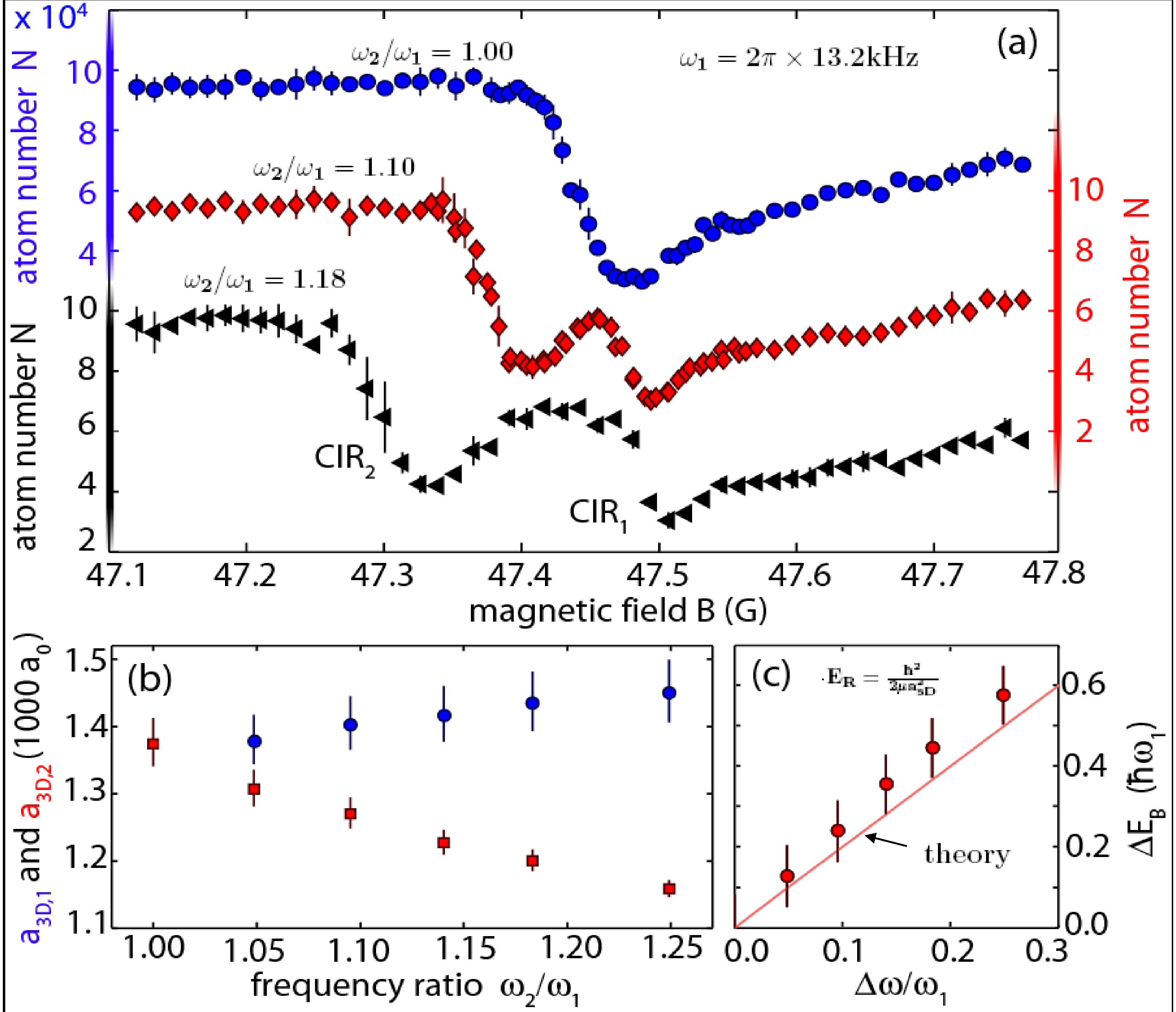
total transmission coefficient T= $\sum W_n T_n$

initial population W_n of the state n={n_1,n_2}

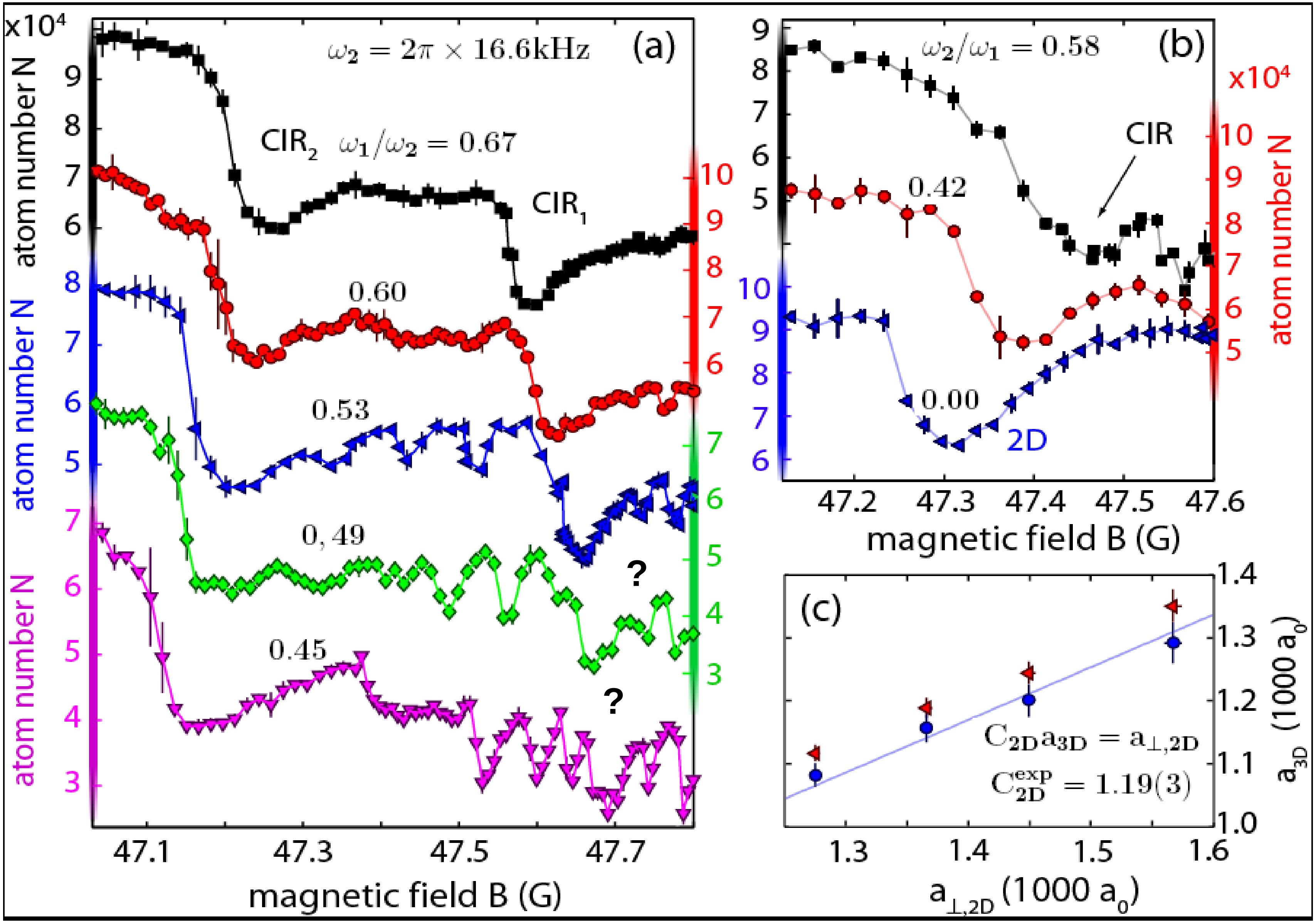
dependence of total transmission coefficient $T(a_\perp/a_s, W_2/W_0)$ on population W_2/W_0



necessary ingredient for the splitting of the minimum of T is a population at least a few percent of the transversally excited state



x 10^4
atom number N
ω2/ω1 = 1.00
ω1 = 2π × 13.2kHz
(a)
ω2/ω1 = 1.10
ω2/ω1 = 1.18
atom number N
CIR2
CIR1
magnetic field B (G)
(b)
a3D,1 and a3D,2 (1000 a0)
frequency ratio ω2/ω1
(c)
theory
ΔEB (ħω1)
Δω/ω1



x10⁴
atom number N
$\omega_2 = 2\pi \times 16.6\text{kHz}$
(a)
CIR₂ $\omega_1/\omega_2 = 0.67$
CIR₁
0.60
0.53
0, 49
0.45
?
?
magnetic field B (G)
$\omega_2/\omega_1 = 0.58$
(b)
x10⁴
CIR
0.42
0.00
2D
magnetic field B (G)
(c)
$C_{2D} a_{3D} = a_{\perp,2D}$
$C_{2D}^{exp} = 1.19(3)$
a_{3D} (1000 a_0)
$a_{\perp,2D}$ (1000 a_0)

no theory !

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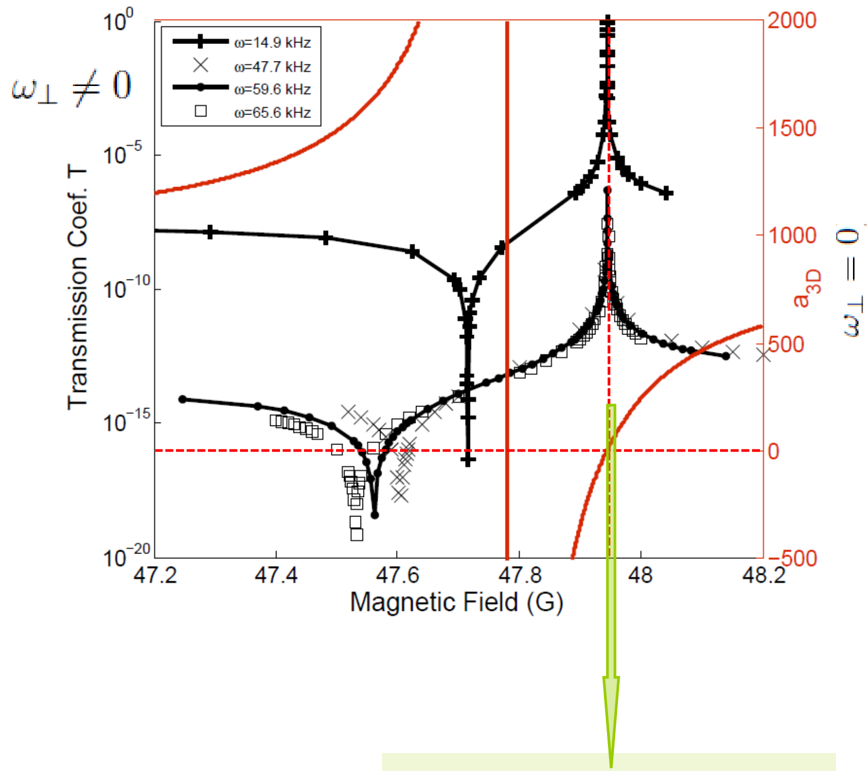

region of Innsbruck experiment
(d-wave Feshbach resonance)

$$\Gamma_i^* = \Delta_i \frac{\sqrt{2E_\parallel}}{\sqrt{\mu} a_{bg} \omega_\perp \gamma_i}$$

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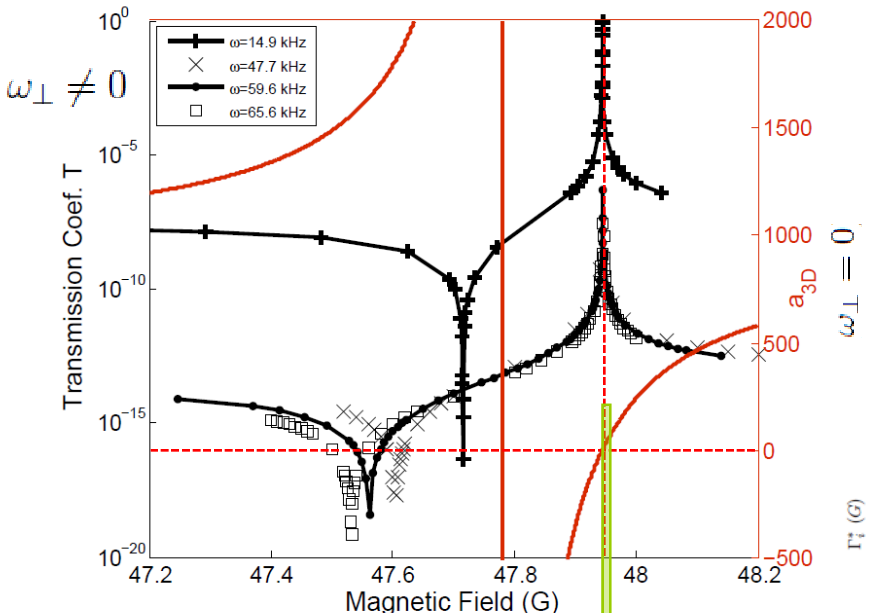

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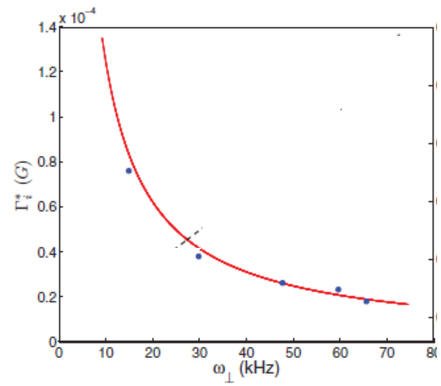

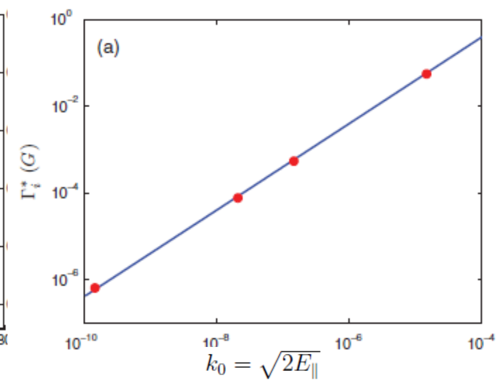

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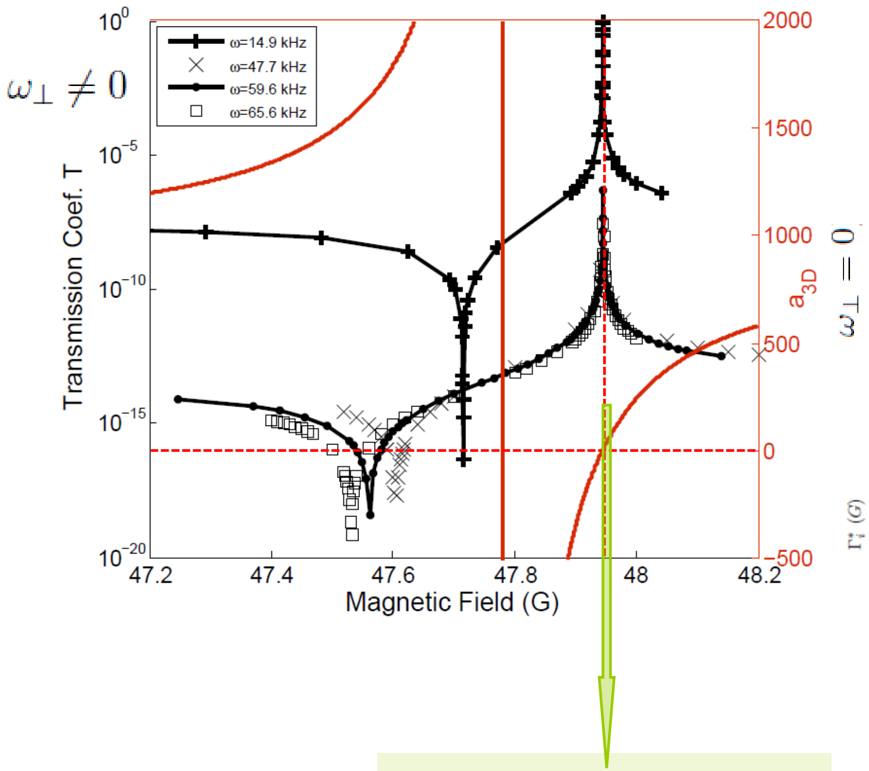

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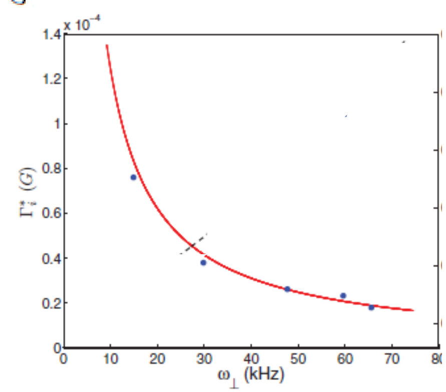
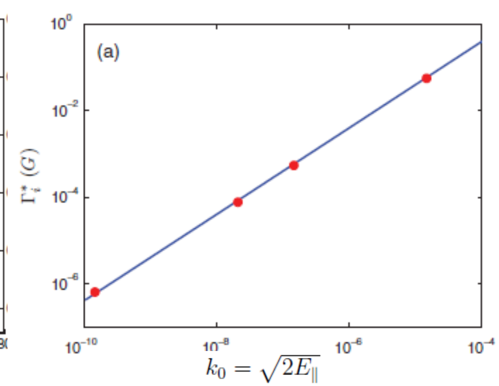




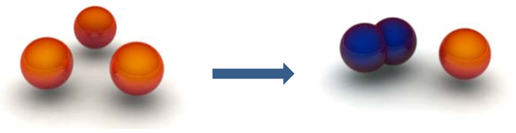
$$\Gamma_i^* = \Delta_i \frac{\sqrt{2E_\parallel}}{\sqrt{\mu} a_{bg} \omega_\perp \gamma_i}$$

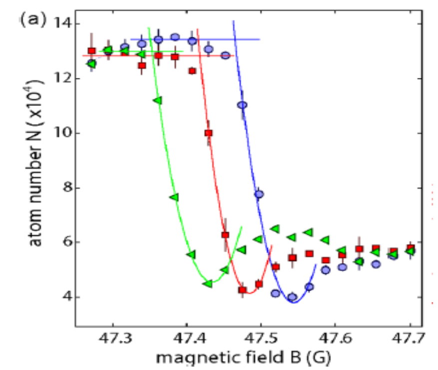
narrowing width Γ^* with increasing $\omega_\perp$

$\Gamma^* \to$ longitudinal temperature $E_\parallel \sim k_B T$

energy release ?

- **triple collisions A + A + A → (AA) + A :**





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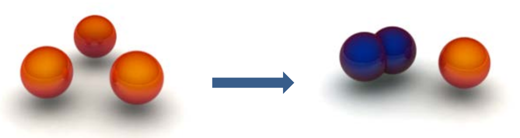

detection of the CIR by anincrease of three-body loss:

E.Haller, M.J. Mark, R. Hart, J.G. Danzl, L. Reichsoellner, V.Melezhik, P. Schmelcher and H.-C. Naegerl, Phys.Rev.Lett. 104 (2010)153203

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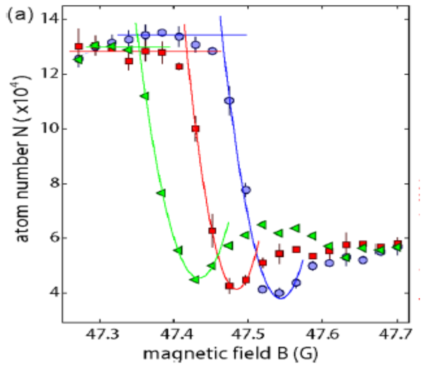

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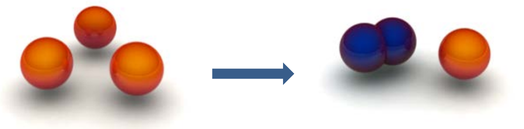

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- **pair collisions with CM excitation** $A_{n1=0}+B_{n2=0} \rightarrow (AB)_{n=0,N=1}$

Mechanism of molecule formation with transferring the energy release to CM excitation of forming molecule was considered in:

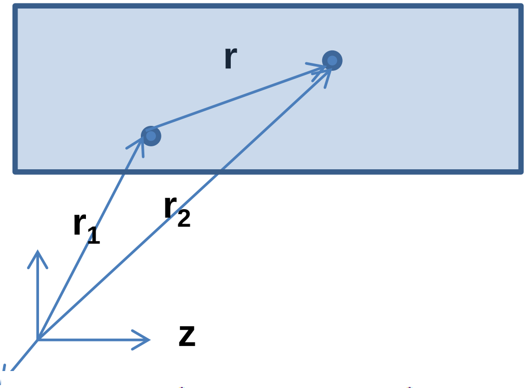
E.Bolda et.al. Phys.Rev. A71,033404 (2004) (in anharmonic lattices)

V.Melezhik &P.Schmelcher, New J.Phys.11,073031 (2009) (distinguishable atoms in harmonic waveguides)

non-separability of two-body problem in trap

(distinguishable atoms in harmonic trap or identical atoms in anharmonic trap)

V. Melezhik & P. Schmelcher, New J. of Phys. 11, 073031 (2009)



$$V(r) + \frac{1}{2} m_1 \omega_1^2 \rho_1 + \frac{1}{2} m_2 \omega_2^2 \rho_2$$

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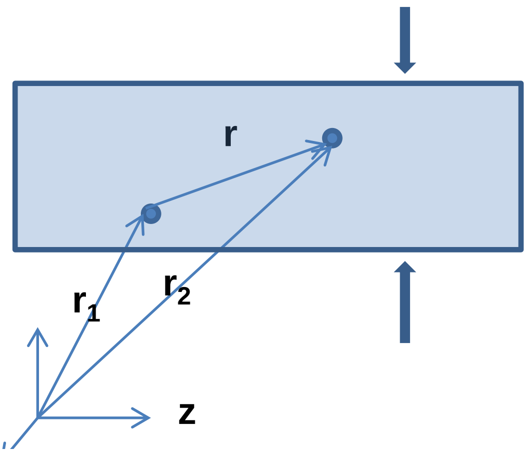

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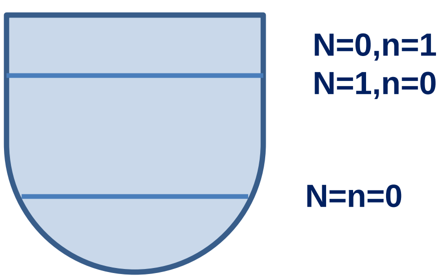

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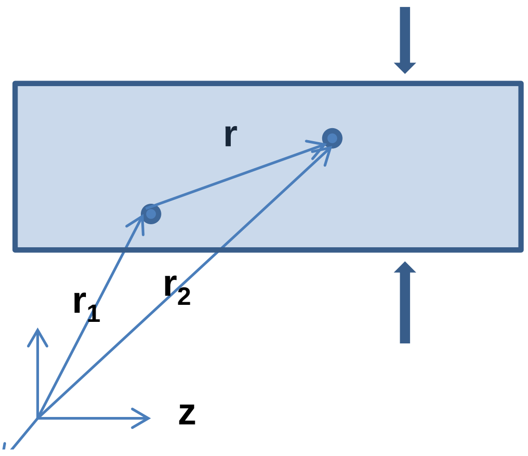
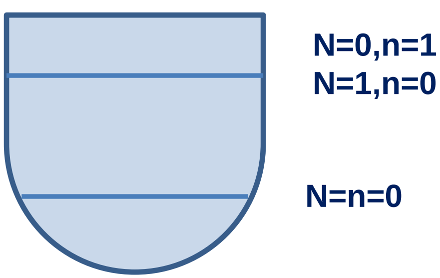


$$V(r) + \tfrac{1}{2} m_1 \omega_1^2 \rho_1 + \tfrac{1}{2} m_2 \omega_2^2 \rho_2$$



$$i \frac{\partial}{\partial t} \psi(\rho_R, \mathbf{r}, t) = H(\rho_R, \mathbf{r}) \psi(\rho_R, \mathbf{r}, t)$$

$$H(\rho_R, \mathbf{r}) = H_{\rm CM}(\rho_R) + H_{\rm rel}(\mathbf{r}) + W(\rho_R, \mathbf{r})$$

$$H_{\rm CM} = -\frac{1}{2M} \left(\frac{\partial^2}{\partial \rho_R^2} + \frac{1}{\rho_R^2} \frac{\partial^2}{\partial \phi^2} + \frac{1}{4\rho_R^2} \right) + \frac{1}{2}(m_1 \omega_1^2 + m_2 \omega_2^2) \rho_R^2$$

$$H_{\rm rel} = -\frac{1}{2\mu} \frac{\partial^2}{\partial r^2} + \frac{L^2(\theta,\phi)}{2\mu r^2} + \frac{\mu^2}{2} \left(\frac{\omega_1^2}{m_1} + \frac{\omega_2^2}{m_2} \right) \rho^2 + V(r)$$

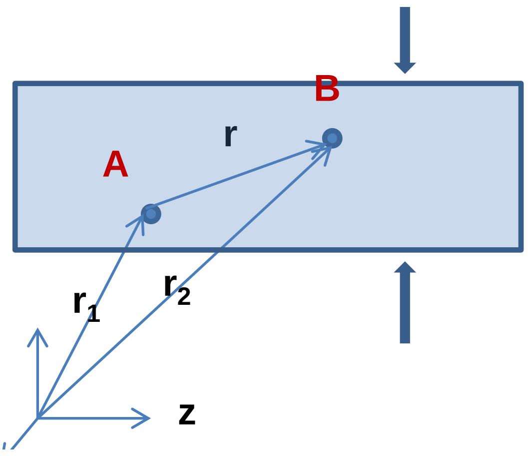
$$\frac{L^2(\theta,\phi)}{2\mu r^2} = -\frac{1}{2\mu r^2 \sin\theta} \left(\frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin\theta} \frac{\partial^2}{\partial \phi^2} \right)$$

$$W(\rho_R, \mathbf{r}) = \mu(\omega_1^2 - \omega_2^2) r \rho_R \sin\theta \cos\phi$$

→ **4D TDSE:** ρ_R, r, θ, ϕ

non-separability of two-body problem in trap
(distinguishable atoms in harmonic trap or identical atoms in anharmonic trap)

V. Melezhik & P. Schmelcher, New J. of Phys. 11, 073031 (2009)



$$V(r) + \tfrac{1}{2}m_1\omega_1^2\rho_1 + \tfrac{1}{2}m_2\omega_2^2\rho_2$$

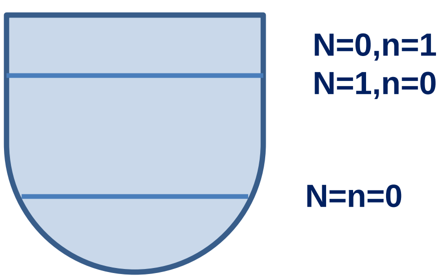
$$i\frac{\partial}{\partial t}\psi(\rho_R,\mathbf{r},t) = H(\rho_R,\mathbf{r})\psi(\rho_R,\mathbf{r},t)$$

$$H(\rho_R,\mathbf{r}) = H_{\mathrm{CM}}(\rho_R) + H_{\mathrm{rel}}(\mathbf{r}) + W(\rho_R,\mathbf{r})$$

$$H_{\mathrm{CM}} = -\frac{1}{2M}\left(\frac{\partial^2}{\partial\rho_R^2} + \frac{1}{\rho_R^2}\frac{\partial^2}{\partial\phi^2} + \frac{1}{4\rho_R^2}\right) + \frac{1}{2}(m_1\omega_1^2 + m_2\omega_2^2)\rho_R^2$$

$$H_{\mathrm{rel}} = -\frac{1}{2\mu}\frac{\partial^2}{\partial r^2} + \frac{L^2(\theta,\phi)}{2\mu r^2} + \frac{\mu^2}{2}\left(\frac{\omega_1^2}{m_1} + \frac{\omega_2^2}{m_2}\right)\rho^2 + V(r)$$

$$\frac{L^2(\theta,\phi)}{2\mu r^2} = -\frac{1}{2\mu r^2\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin\theta}\frac{\partial^2}{\partial\phi^2}\right)$$



$$W(\rho_R,\mathbf{r}) = \mu(\omega_1^2 - \omega_2^2)r\rho_R\sin\theta\cos\phi$$ → **4D TDSE:** ρ_R, r, θ, ϕ

$A_{n1=0}$ + $B_{n2=0}$ → $(AB)_{n=0,N=1}$

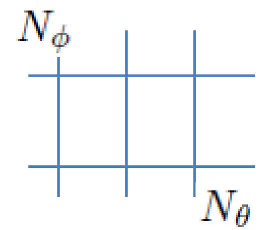
5D TDSE

- **Discretization of the angular subspace:**
  2D nondirect product discrete variable representation (npDVR)

$$\psi(\rho_R, r, \Omega, t) = \sum_{j=1}^{N} f_j(\Omega)\psi_j(\rho_R, r, t) \qquad \sum_{\nu=1}^{N} = \sum_{m=-(N_\phi-1)/2}^{(N_\phi-1)/2} \sum_{l=|m|}^{|m|+N_\theta-1}$$

$$f_j(\Omega) = \sum_{\nu=1}^{N} Y_\nu(\Omega)(Y^{-1})_{\nu j} \qquad \Omega_j = (\theta_{j_\theta}, \phi_{j_\phi})$$

$$Y_\nu(\Omega) = Y_{lm}(\Omega) = e^{im\phi} \sum_{l'} C_l^{l'} \times P_{l'}^m(\theta) \qquad Y_{j\nu} = Y_\nu(\Omega_j)$$



V.Melezhik, Phys.Lett.A230(1997)203
V.Melezhik, AIP Conf.Proc.1479(2012)1200

- **Computational scheme: component-by-component split operator method**

$$i\frac{\partial}{\partial t}\psi_j(\rho_R, r, t) = \sum_{j'}^{N} H_{jj'}(\rho_R, r)\psi_{j'}(\rho_R, r, t) \qquad t_n \to t_{n+1} = t_n + \Delta t$$

interaction is diagonal in ndDVR $f_j(\Omega)$

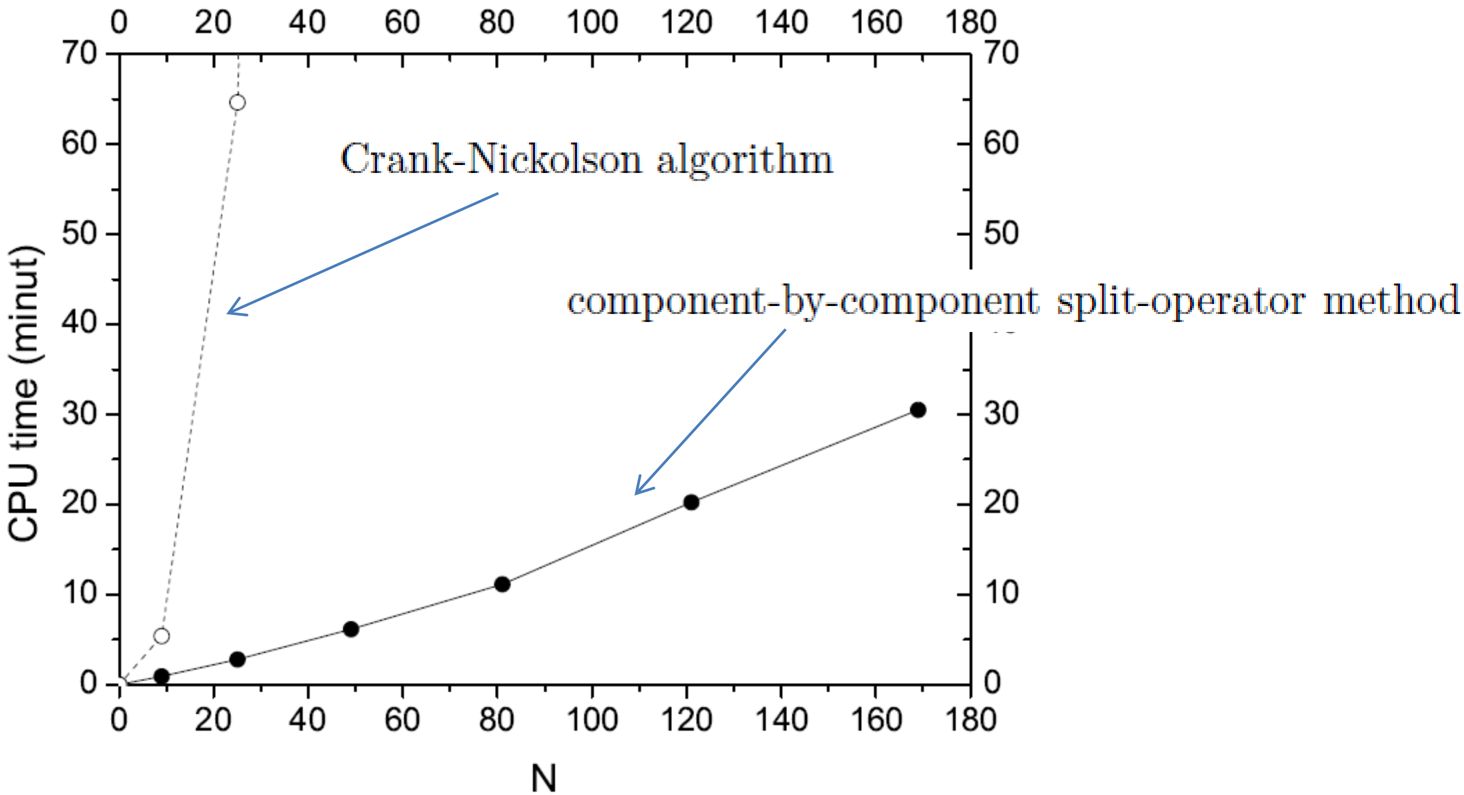
kinetic energy operator is diagonal in $Y_\nu(\Omega) = Y_{lm}(\Omega)$

$$S_{j\nu} = \lambda_j^{1/2} Y_{j\nu}$$

V.Melezhik, Phys.Lett.A230(1997)203
V.Melezhik,J.I.Kim,P.Schmelcher, Phys.Rev.A76(2007)053611

economic computational scheme

V.Melezhik, Phys.Lett.A230(1997)203
V.Melezhik, AIP Conf.Proc.1479(2012)1200
V.Melezhik,J.I.Kim,P.Schmelcher, Phys.Rev.A76(2007)053611



$$\psi(\rho_R, r, \Omega, t) = \sum_{j=1}^{N} f_j(\Omega)\psi_j(\rho_R, r, t) \qquad \sum_{\nu=1}^{N} = \sum_{m=-(N_\phi-1)/2}^{(N_\phi-1)/2} \sum_{l=|m|}^{|m|+N_\theta-1}$$

BLTP JINR two-core Intel processor Xenon 5160 with 3GHz frequency

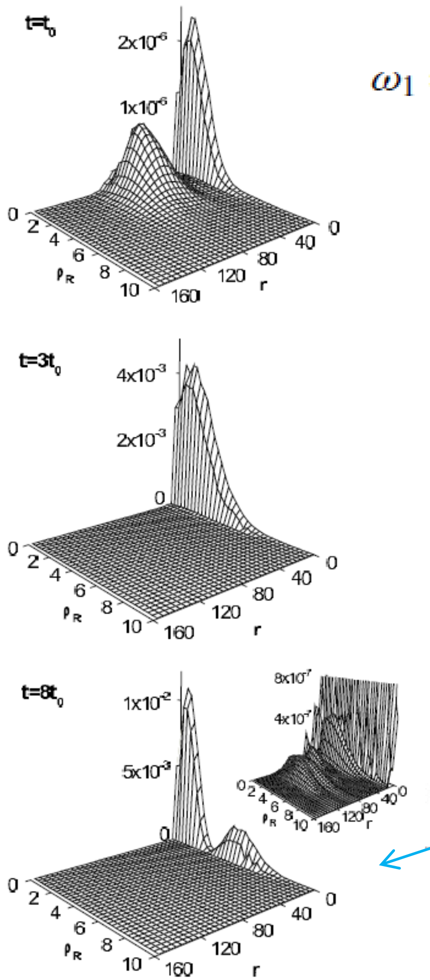
$A_{n1=0}$ + $B_{n2=0}$ → $(AB)_{n=0,N=1}$

Time evolution of the probability density distribution during collision

$$W(\rho_R, r, t) = \int |\psi(\rho_R, r, \theta, \phi, t)|^2 (r^2 \rho_R)^{-1} \sin\theta \, d\theta \, d\phi$$

CM coupling with interatomic motion:

$$\omega_1 \neq \omega_2$$



molecule formation

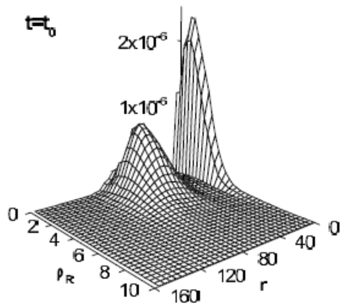
$A_{n1=0} + B_{n2=0} \rightarrow (AB)_{n=0,N=1}$

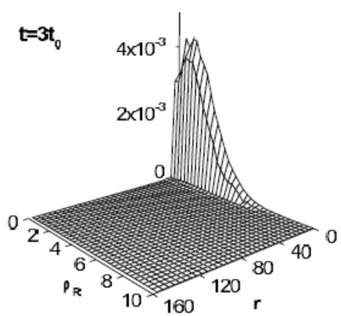
Time evolution of the probability density distribution during collision

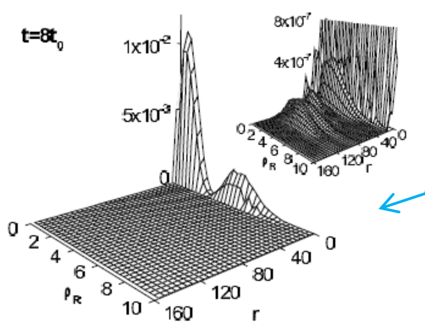
$$W(\rho_R, r, t) = \int |\psi(\rho_R, r, \theta, \phi, t)|^2 (r^2 \rho_R)^{-1} \sin\theta \, d\theta \, d\phi$$

CM coupling with interatomic motion:

$\omega_1 \neq \omega_2$



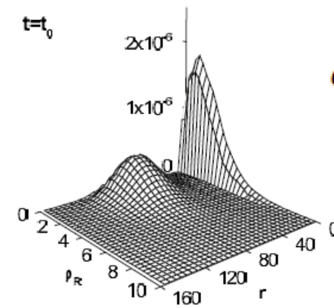


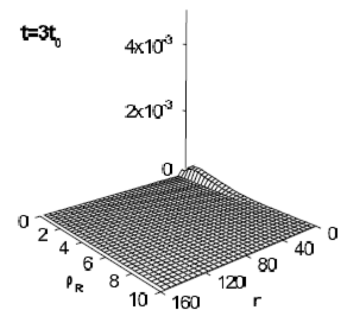


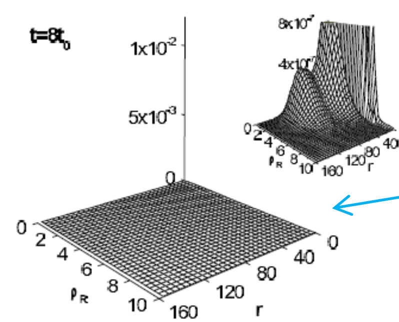
molecule formation

CM decouples from interatomic motion:

$\omega_1 = \omega_2$







no molecule

Resonant Formation of Ultracold Molecules in Waveguides

V. Melezhik & P. Schmelcher, New J. of Phys. 11, 073031 (2009)

coupling of the deatomic continuum with the CM of excited molecule at (N=1) in closed transverse channels:

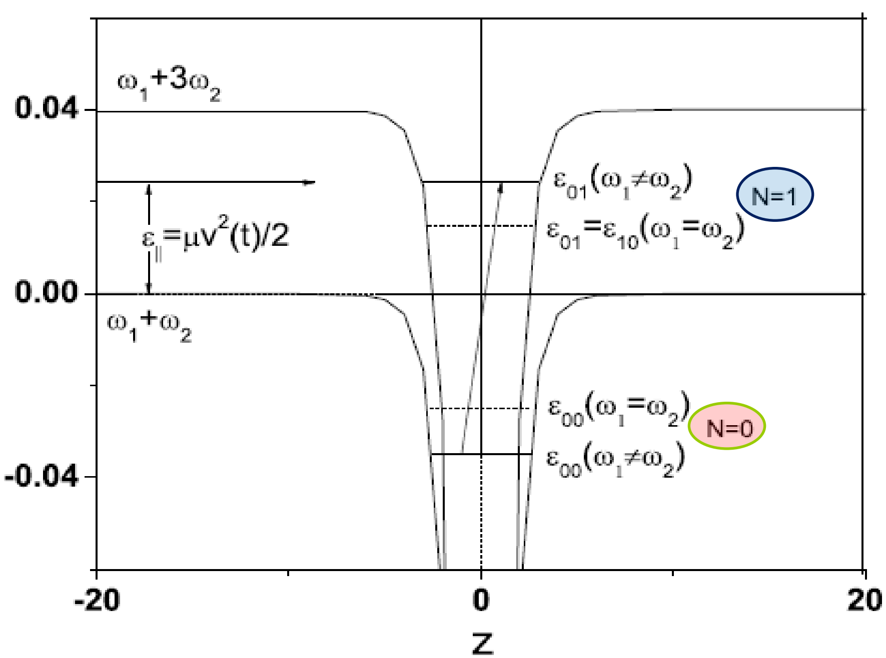
$$W(\rho_R, \boldsymbol{r}) = \mu\,(\omega_1^2 - \omega_2^2)\, r\,\rho_R \sin\theta\cos\phi$$

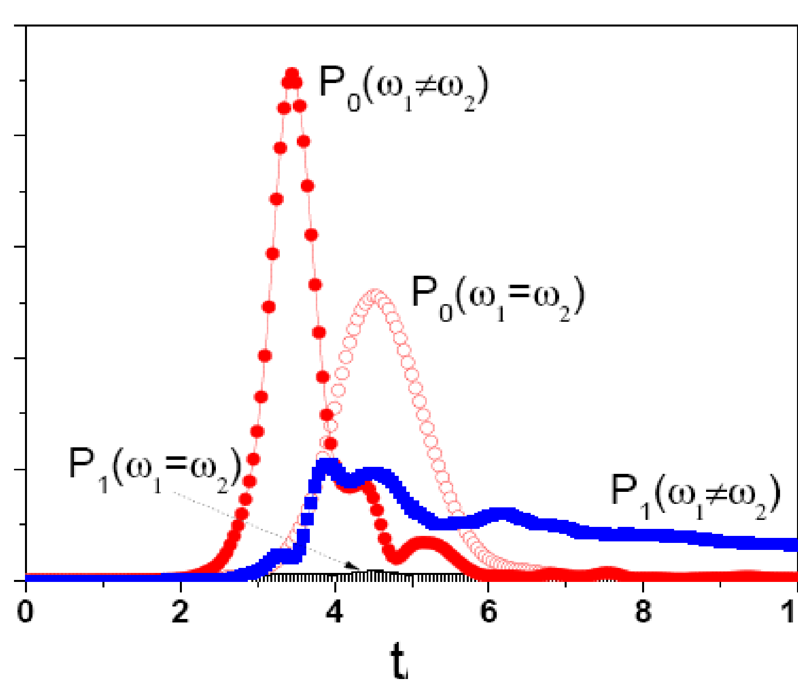
if the atoms in the colliding pair are identical, then coupling term goes to zero and the effect disappears.

TDSE: 4D

$A_{n1=0}$ + $B_{n2=0}$ → $(AB)_{n=0,N=1}$

Time evolution of the molecular states (N=0 and 1) population $P_N(t)$ during a pair collision:





in Heidelberg experiment , S.Sala et. al. Phys.Rev.Lett.110,203202 (2013),
the mechanism of molecule formation with transferring
energy release to CM molecule excitation was observed
in anharmonic waveguide

Dipolar confinement-induced resonances in waveguides

P.Giannakeas, V. Melezhik & P.Schmelcher, PRL,111(2013)

$$\vec{d} \quad \vec{d}$$

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + \underbrace{\frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}}_{V_{sr}} + \underbrace{\frac{d^2}{r^3}[1 - 3(\hat{z}\cdot\hat{r})]}_{V_{dd}}$$

$$\downarrow$$

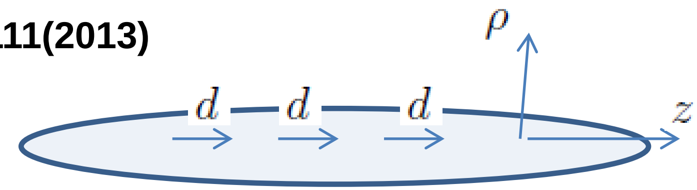
$$\underline{K}^{3\mathrm{D}} = \begin{pmatrix} K_{ss} & K_{sd} & 0 \\ K_{ds} & K_{dd} & K_{dg} \\ 0 & K_{gd} & K_{gg} \end{pmatrix}$$

$$a_{ll'} = -\frac{K_{ll'}}{k}$$

$$l_d = \frac{\mu d^2}{\hbar^2}$$

Dipolar confinement-induced resonances in waveguides

P.Giannakeas, V. Melezhik & P.Schmelcher, PRL,111(2013)



$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{\mu}{2}\omega_\perp^2\rho^2 + \underbrace{\frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}}_{V_{sr}} + \underbrace{\frac{d^2}{r^3}[1-3(\hat{z}\cdot\hat{r})]}_{V_{dd}}$$

$$a_\perp = \sqrt{\frac{\hbar}{\mu\omega_\perp}}$$

$$\underline{\tilde{K}}_{oo}^{1D} = \underline{K}_{oo}^{1D} + i\underline{K}_{oc}^{1D}(\mathcal{I} - i\underline{K}_{cc}^{1D})^{-1}\underline{K}_{co}^{1D}$$

$$\underline{K}^{3\mathrm{D}} = \begin{pmatrix} K_{ss} & K_{sd} & 0 \\ K_{ds} & K_{dd} & K_{dg} \\ 0 & K_{gd} & K_{gg} \end{pmatrix}$$

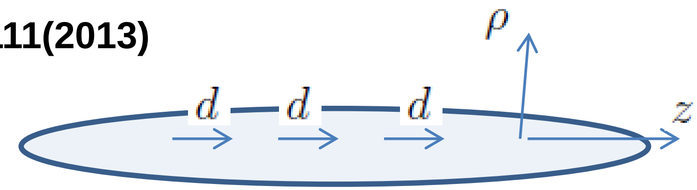
$$\det(\mathcal{I} - i\underline{K}_{cc}^{1D}) = 0$$

$$a_{ll'} = -\frac{K_{ll'}}{k} \qquad \bar{a}_{ll'} = \frac{a_{ll'}}{a_\perp}$$

$$l_d = \frac{\mu d^2}{\hbar^2} \qquad \bar{l}_d = \frac{l_d}{a_\perp}$$

Dipolar confinement-induced resonances in waveguides

P.Giannakeas, V. Melezhik & P.Schmelcher, PRL,111(2013)



$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{\mu}{2}\omega_\perp^2\rho^2 + \underbrace{\frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}}_{V_{sr}} + \underbrace{\frac{d^2}{r^3}[1-3(\hat{z}\cdot\hat{r})]}_{V_{dd}}$$

$$a_\perp = \sqrt{\frac{\hbar}{\mu\omega_\perp}}$$

$$\underline{\tilde{K}}_{oo}^{1D} = \underline{K}_{oo}^{1D} + i\underline{K}_{oc}^{1D}(\mathcal{I} - i\underline{K}_{cc}^{1D})^{-1}\underline{K}_{co}^{1D}$$

$$\underline{K}^{3D} = \begin{pmatrix} K_{ss} & K_{sd} & 0 \\ K_{ds} & K_{dd} & K_{dg} \\ 0 & K_{gd} & K_{gg} \end{pmatrix}$$

$$\det(\mathcal{I} - i\underline{K}_{cc}^{1D}) = 0$$

$$a_{ll'} = -\frac{K_{ll'}}{k} \qquad \bar{a}_{ll'} = \frac{a_{ll'}}{a_\perp}$$

we obtained resonance condition:

$$\bar{a}_{ss}(ka_\perp, d) = \mathcal{F}(\{\bar{a}_{\ell\ell'}(ka_\perp, d)\})$$

$$l_d = \frac{\mu d^2}{\hbar^2} \qquad \bar{l}_d = \frac{l_d}{a_\perp}$$

$$\mathcal{F}_{\mathrm{BA}} = -\frac{1 + \eta_1\bar{l}_d + \eta_2\bar{l}_d^2 + \eta_3\bar{l}_d^3}{\sigma_0 + \sigma_1\bar{l}_d + \sigma_2\bar{l}_d^2}$$

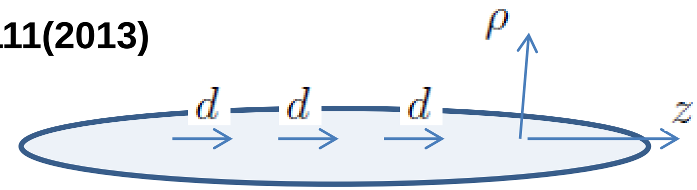
For $l_d = 0$, the resonance condition $\bar{a}_{ss} = \mathcal{F}_{\mathrm{BA}}$

reduces to $\bar{a}_s = -1/\sigma_0 = 0.68$

$$a_s = 0.68a_\perp$$

Dipolar confinement-induced resonances in waveguides

P.Giannakeas, V. Melezhik & P.Schmelcher, PRL,111(2013)



$$l_{vdW} = \left(\frac{2\mu C_6}{\hbar^2}\right)^{1/4}$$

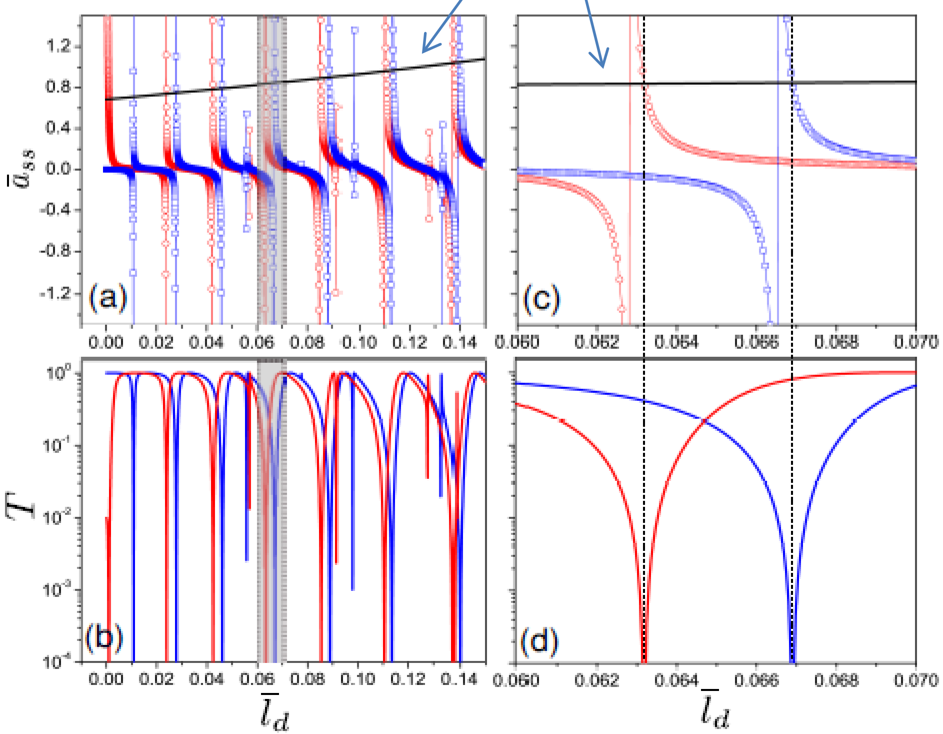
$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{\mu}{2}\omega_\perp^2\rho^2 + \underbrace{\frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}}_{V_{sr}} + \underbrace{\frac{d^2}{r^3}[1 - 3(\hat{z}\cdot\hat{r})]}_{V_{dd}}$$

$$a_\perp = \sqrt{\frac{\hbar}{\mu\omega_\perp}}$$

$a_s \gg l_{\mathrm{vdW}}$ (—○—)

$a_s \ll l_{\mathrm{vdW}}$ (—□—)

$$\mathcal{F}_{\mathrm{BA}} = -\frac{1 + \eta_1\bar{l}_d + \eta_2\bar{l}_d^2 + \eta_3\bar{l}_d^3}{\sigma_0 + \sigma_1\bar{l}_d + \sigma_2\bar{l}_d^2}$$



$$\bar{a}_{ll'} = \frac{a_{ll'}}{a_\perp} \qquad a_{ll'} = -\frac{K_{ll'}}{k}$$

$$\bar{l}_d = \frac{l_d}{a_\perp} \qquad l_d = \frac{\mu d^2}{\hbar^2}$$

For $l_d = 0$, the resonance condition $\bar{a}_{ss} = \mathcal{F}_{\mathrm{BA}}$ reduces to $\bar{a}_s = -1/\sigma_0 = 0.68$

$$a_s = 0.68 a_\perp$$

$$T = \frac{1}{1 + \frac{\mu^2 g_{1D}^2}{\hbar^4 q_0^2}} = \frac{1}{1 + (\tilde{K}_{oo}^{1D})^2}$$

Quantum simulation with fully controlled few-body systems

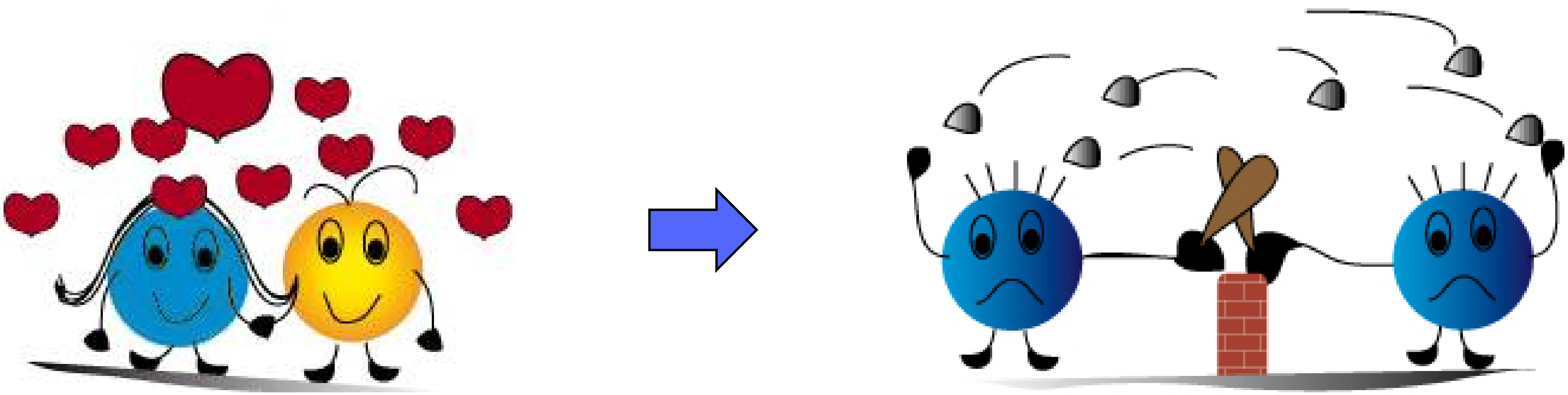
control over: quantum states

particle number

interaction

G.Zurn et. al. Phys. Rev. Lett. 108, 075303 (2012)

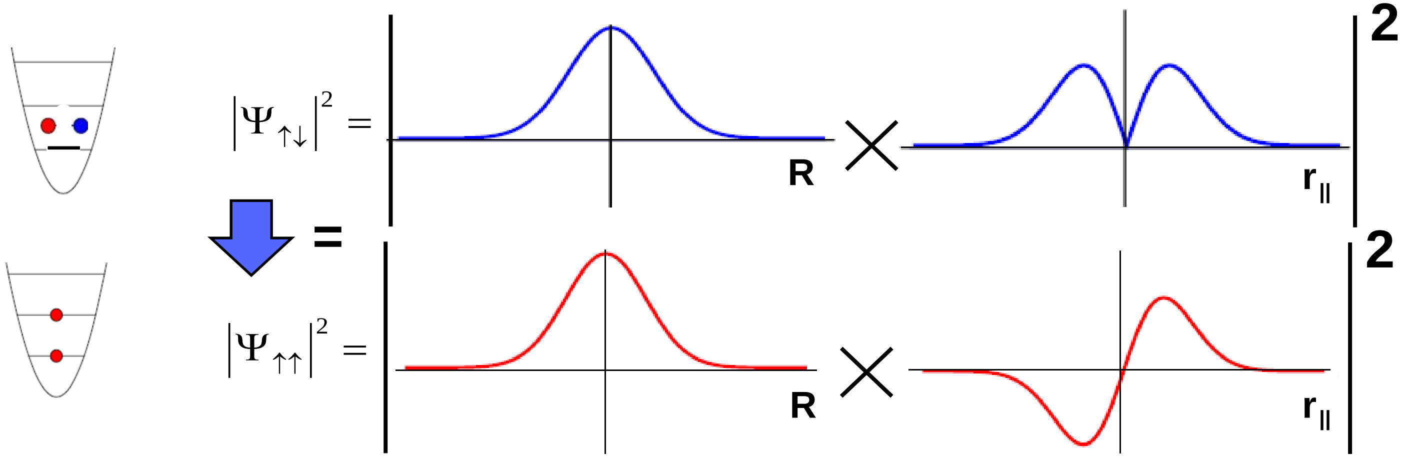
Fermionization of two distinguishable Fermions



G.Zurn et. al. Phys. Rev. Lett. 108, 075303 (2012)

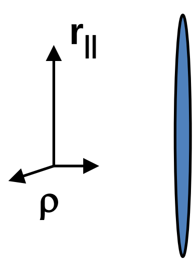
image source: MPG

Mappin $g_{1D} \to \pm\infty$

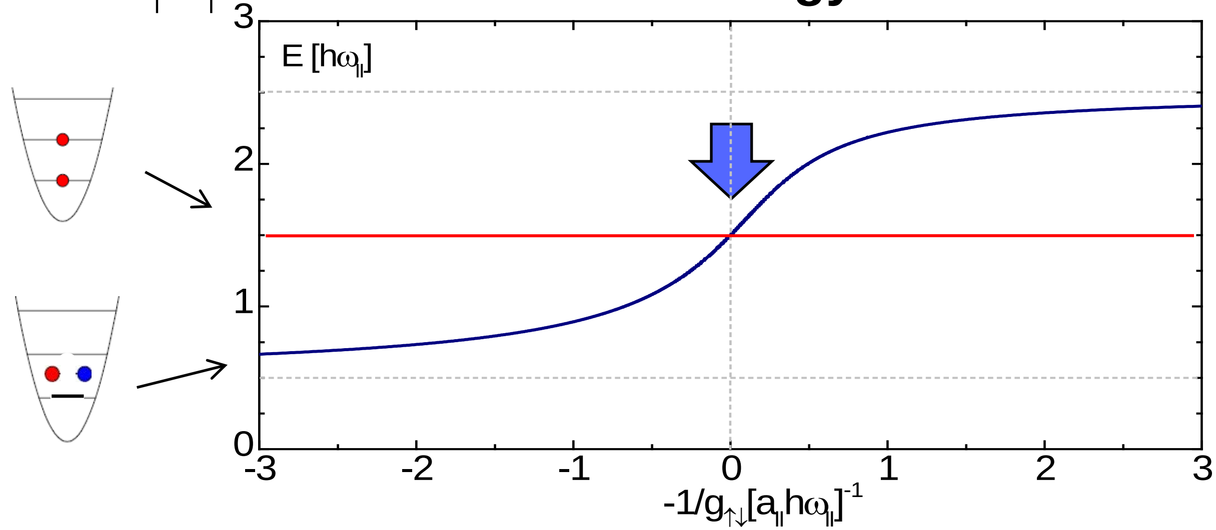


M.D. Girardeau, PRA 82, 011607(R) (2010)

in 1D:



same $|\Psi|^2$ ⟷ same energy



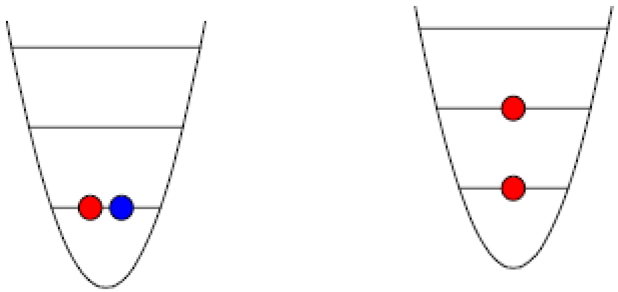
$g_{1D} > 0$ $g_{1D} \to \pm\infty$ $g_{1D} < 0$

analytic solution for energy:

T. Busch et al., Found Phys Vol.28, No.4 549-559 (1998)

How one can measure this?

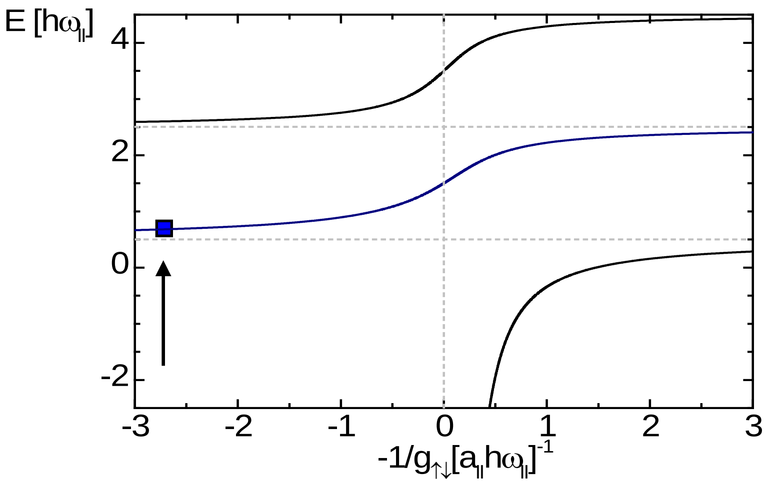
- Prepare the systems with high fidelity in the ground state

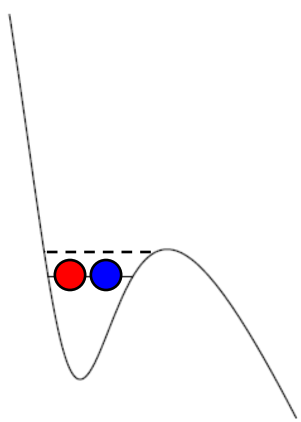


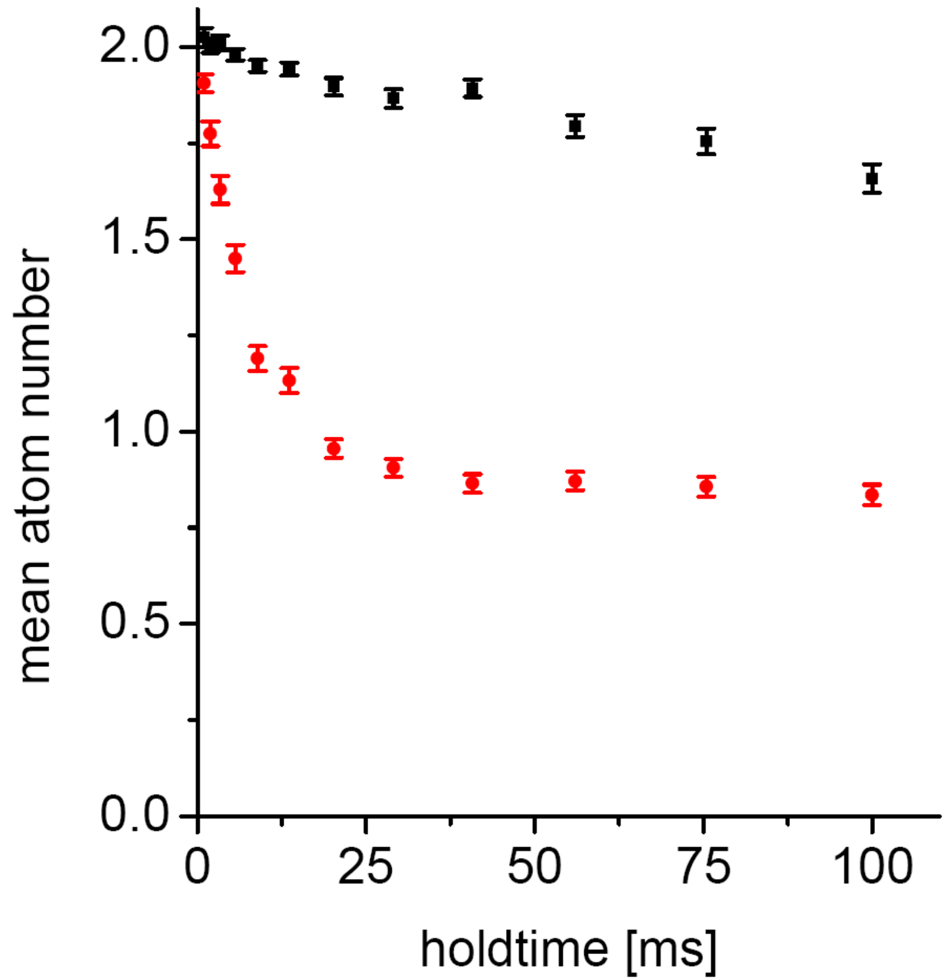
- modify the interaction strength

- measure the energy of the systems

Measurement of the energy: Tunneling with interaction



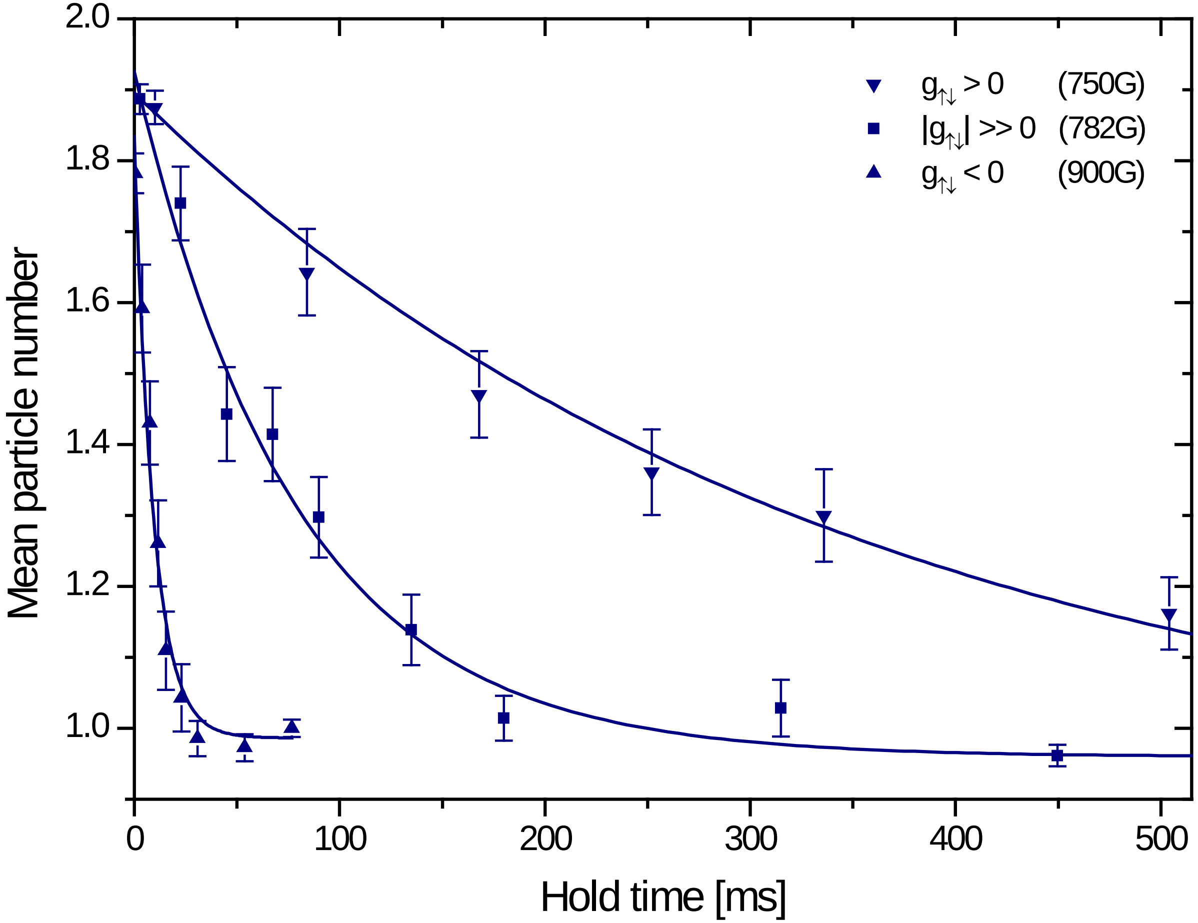




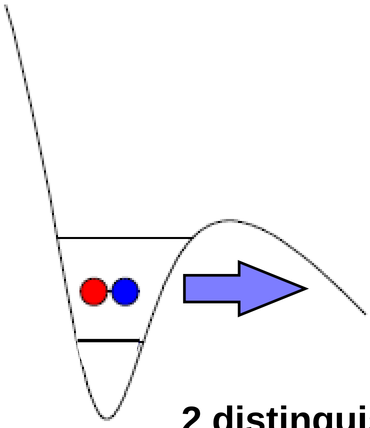
G.Zurn et. al. Phys. Rev. Lett. 108, 075303 (2012)

Determine tunneling time

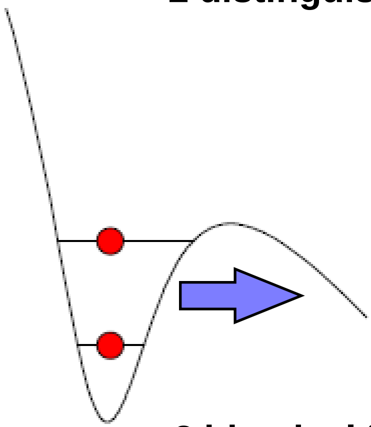
fixed barrier height, different magnetic field values



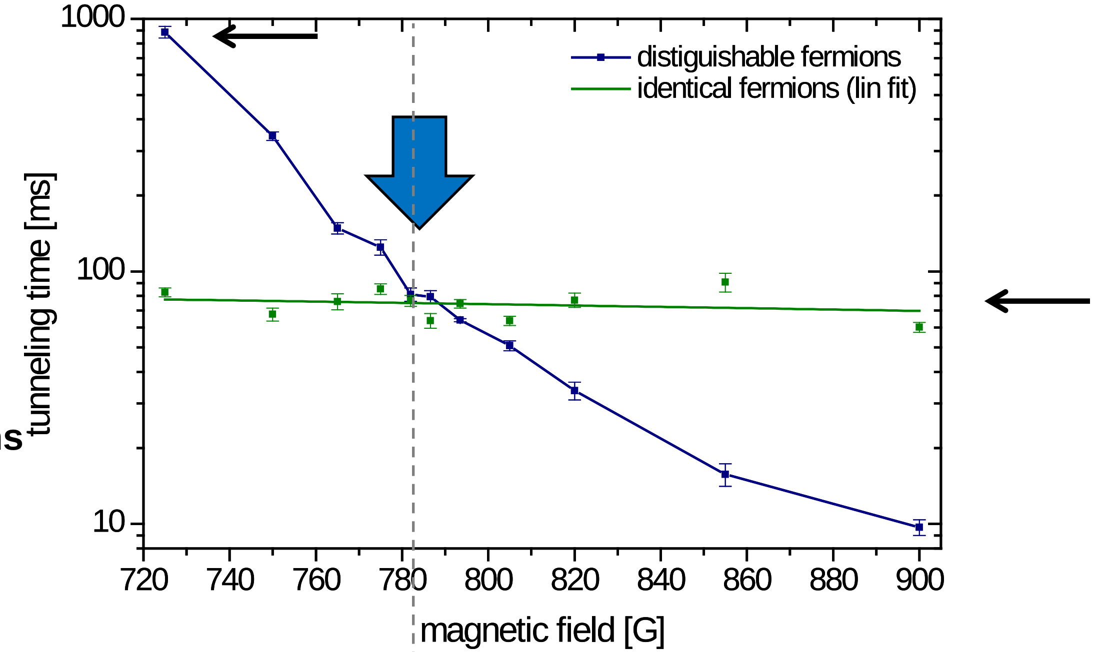
G.Zurn et. al. Phys. Rev. Lett. 108, 075303 (2012)

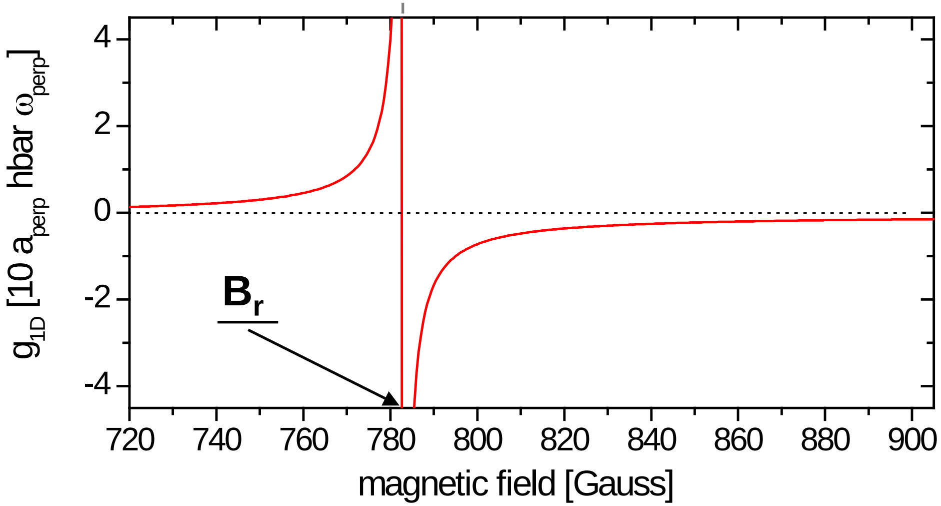


2 distinguishable fermions



2 identical fermions

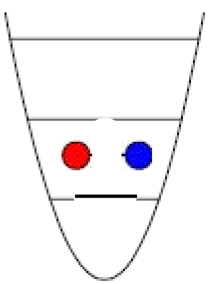




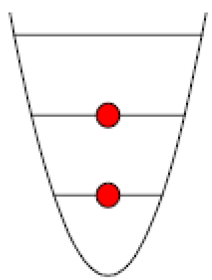
$a_{3D}(B_r)/a_L = 1.46$ <-- CIR !!!

- **Same tunneling time → Same energy**
- **Same energy → in 1D only one unique solution for the wavefunction square**

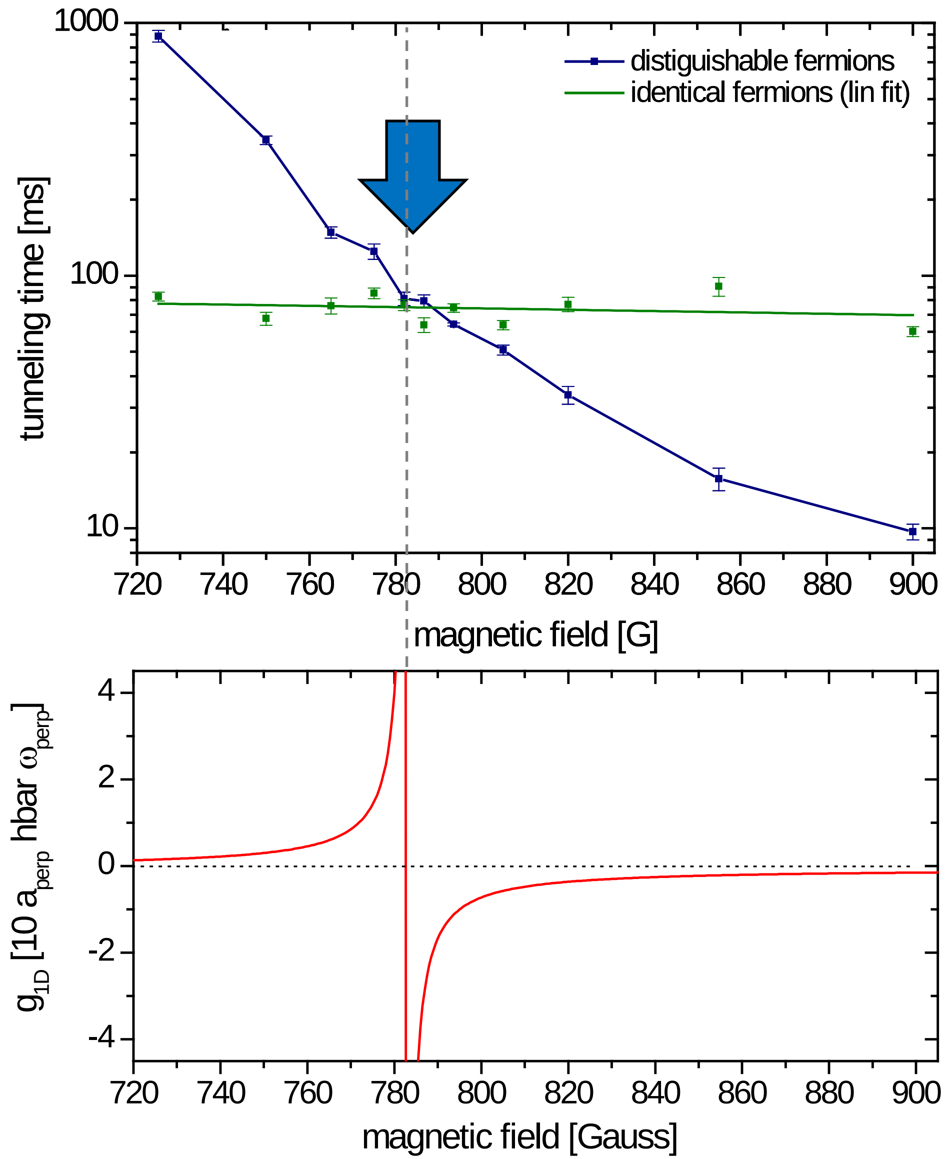
→ Experimental proof of the mapping:



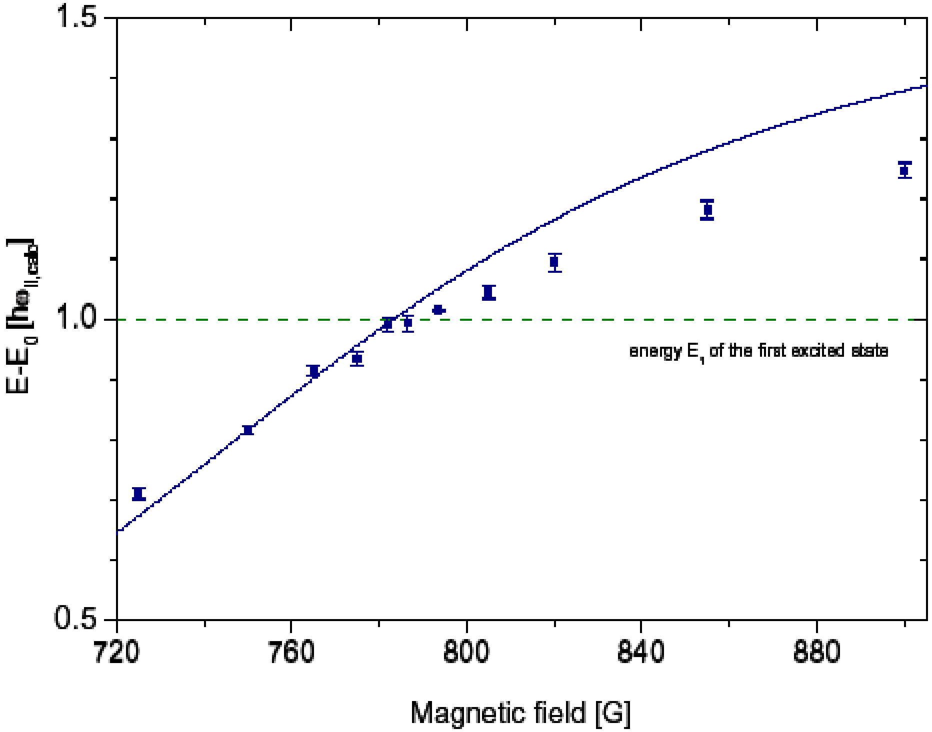
behaves like



Fermionisation of two distinguishable fermions



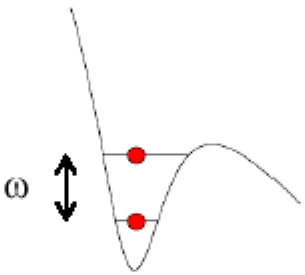
Deduce energy from tunneling time



WKB: Determination of the potential

- Tunneling exponentially sensitive to potential shape
- Calibration of the potential
- Obtain energies from tunneling time

Compare to theory for harmonic trap



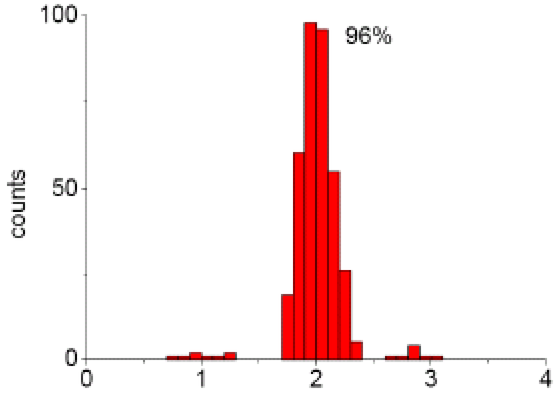
- Improvement: theory of Quasi-particle tunneling

M.Rontani, arXiv: 1111.3611

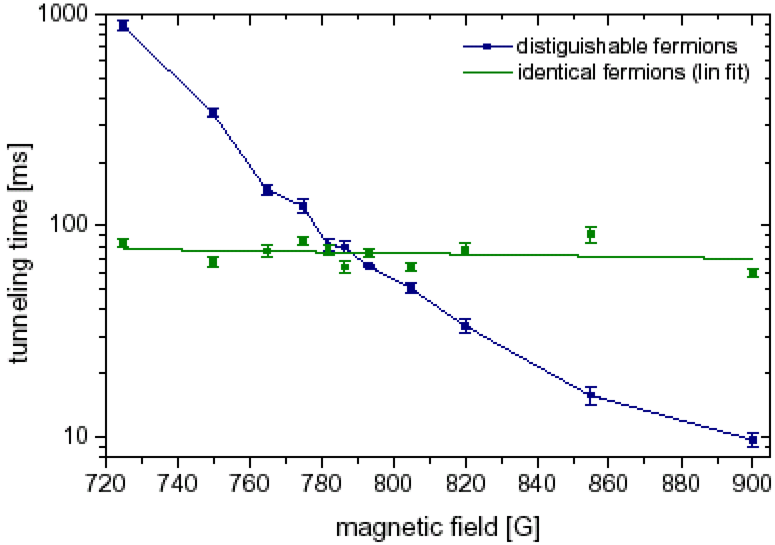
Conclusion

Achievement:

- few-particle systems in well defined quantum states



- Control over the interaction strength of 2 particles



- Tested various spectroscopic methods

Opened the door for Quantum simulation of few body systems

G.Zurn et. al. Phys. Rev. Lett. 108, 075303 (2012)

Experimental setups in:

MIT (Boston), Boulder, NIST (Washington), Munich, Heidelberg, Shtutgart, Hamburg, Innsbruck, Vienna, Paris, Firenze, Barselona, N.Novgorod, Troitsk …

Rb,Cs,K,Sr,Li …

Rb_2 , Cs_2 , RbK … **1D, 2D, 3D**

~ 80 experimental groups worldwide

time of simple models is over

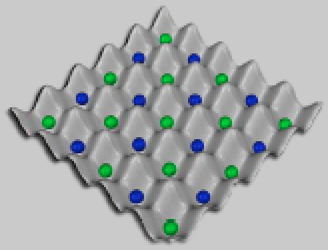
Quantum simulation with fully controlled few-body systems

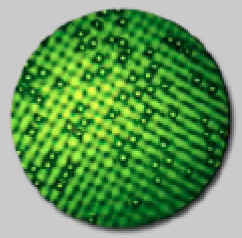
control over: quantum states, particle number, interaction

- attractive interactions ➡ BCS-like pairing in finite systems
- repulsive int.+splitting of trap ➡ entangled pairs of atoms
  (quantum information processing)
- + periodic potential ⟶ quantum many-body physics
  (systems with low entropy to explore
  such as quantum magnetism)
- ...

From Artificial Quantum Matter to Real Materials

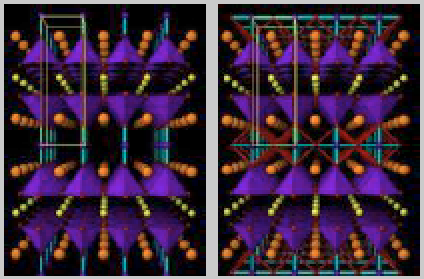
Ultracold Quantum Gases in Optical Lattices





- **Densities:** $10^{14}/cm^3$
(100000 times thinner than air)
- **Temperatures:** few nK
(100 millionen times lower than outer space)
- **Crystal Structures and Material Parameters can be changed dynamically and in-situ.**

Real Materials



e.g. High-T_c Superconductors (YBCO)

- **Densities:** 10^{24}-$10^{25}/cm^3$
- **Temperatures:** mK – several hundred K
- **Crystal Structures and Material Parameters given by Material**
(Tuning possible via e.g. external parameters like e.g. pressure, B-fields or via synthesis)

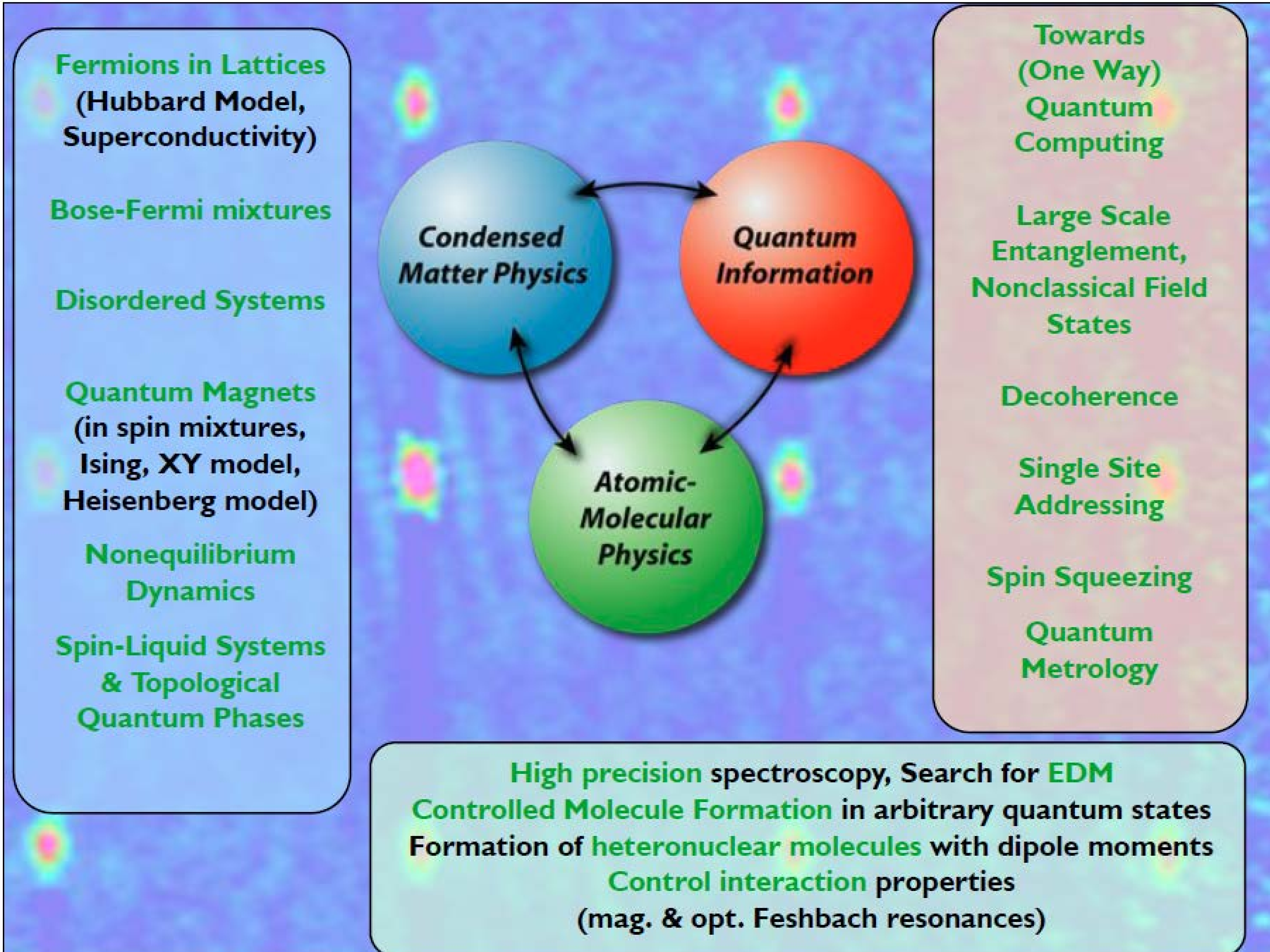
New tunable model systems for many body systems!

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

R. P. Feynman's Vision

A Quantum Simulator to study the quantum dynamics of another system.

R.P. Feyman, Int. J. Theo. Phys. (1982)
R.P. Feynman, Found. Phys (1986)


Fermions in Lattices
(Hubbard Model,
Superconductivity)
Bose-Fermi mixtures
Disordered Systems
Quantum Magnets
(in spin mixtures,
Ising, XY model,
Heisenberg model)
Nonequilibrium
Dynamics
Spin-Liquid Systems
& Topological
Quantum Phases
Condensed
Matter Physics
Quantum
Information
Atomic-
Molecular
Physics
Towards
(One Way)
Quantum
Computing
Large Scale
Entanglement,
Nonclassical Field
States
Decoherence
Single Site
Addressing
Spin Squeezing
Quantum
Metrology
High precision spectroscopy, Search for EDM
Controlled Molecule Formation in arbitrary quantum states
Formation of heteronuclear molecules with dipole moments
Control interaction properties
(mag. & opt. Feshbach resonances)

Results were obtained in collaboration with

Peter Schmelcher (ZOQ,Hamburg)

Panagiotis Giannakeas (ZOQ,Hamburg)

Shahpoor Saeidian (IASBS,Zanjan,Iran)

Innsbruck experiment:

Elmar Haller

Hans-Chrisroph Nägerl